IMACS2023

21st IMACS World Congress

SEPTEMBER 11 - 15, 2023

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Civil and Industrial Engineering Faculty
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Editors: Sandra Carillo
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IMACS2023

Book of Abstracts of IMACS2023
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September 11 - 15, 2023

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Sandra Carillo, Costanza Conti,
Daniela Mansutti, Francesca Pitolli,
Rosa Maria Spitaleri

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About *IMACS*

International Association for
Mathematics and Computers in Simulation

The history

The beginnings of IMACS dated from 1955, when an International Conference on Analog Computation was held at the Brussels Free University (ULB), attended by scientists and managers of simulation laboratories from different countries of the world. Many of these laboratories were by-products of the enormous technological developments that had been brought about by World War II. The participation was truly international, with attendees coming from most European countries including Russia, the United States of America, Japan.

During the conference, it was realized that there was a need for establishing some permanent means of communication between the members of such a new scientific community. This resulted in the creation of AICA (the International Association for Analogue Computation) which was legally incorporated under the Belgian Law in 1956.

The birth of AICA exhibited the emergence, at that time, of disciplines spurred by new technologies, in particular those resulting in tools having to do with the mechanization of information and computation. The example was followed by other organizations in particular fields of applications, namely IFAC (Automatic Control, 1957), IFORS (Operations Research-1959), IMEKO (Measurement – 1959) and IFIP (Information Processing-1960).

In 1972, these five organizations decided to coordinate their activities with the creation of FIACC (the Five International Associations Coordinating Committee), which was created with the support of UNESCO.

It had been under Jean Hoffmann, Professor at the Brussels Free University (ULB), that the 1955 International Conference on Analog Computation, giving birth to AICA, was organized. He became President of the newborn association, a post he held until 1973.

The objectives of AICA remained pretty much unchanged during that period, objectives related to analog computation developed as a tool for applications to mostly industrial problems. This included hardware questions, mathematical and programming aspects with some consideration, beginning in the mid-

1960's, to what had emerged as hybrid computing, i.e. computing involving linked analog and digital machines.
After Hoffmann, Professor Robert Vichnevetsky was elected President at the AICA's 7th World Congress in Prague, August 1973. It was during Vichnevetsky's tenure that the Association grew, reaching the visibility it holds today in scientific computing and applied mathematics. Significant developments were taking place in the sciences at the time and the scope of what was still known as AICA began to expand to include numerical computing, subdisciplines in applied mathematics, and the introduction of mathematical modeling in many of the traditional fields of the applied sciences that had to change their ways to keep up with the new environment. In 1976, AICA changed its name to IMACS (International Association for Mathematics and Computers in Simulation) to reflect the widening of its areas of interests.

Disciplinary directions

The post World War II years had been characterized by significant changes in sciences and industry, brought about by what has come to be called the 'computer revolution', the mechanization of computation and information processing. There had been modest beginnings in earlier times (to which the names of Pascal, Leibniz, Jacquard, Babbage, Kelvin, Hollerith and others are attached in historical reconstructions), but it was not until the middle of the 20th century that computers and the many ramifications related to the theoretical tools needed for their applications became a field of their own, with research, funding and industrial development to back it up. Significant communities of scientists, engineers, technicians engaged in these developments appeared in developed countries throughout the world.
One of the earliest class of scientific problems solved by machines was that of computing the dynamics of mechanical and similar systems, those described with differential equations. Analog computers achieving this had been built since the 1930's (Vannevar Bush at the MIT). ENIAC, the first significant digital computer– built at the University of Pennsylvania during the war years (Eckert, Mauchly, with a significant participation by von Neumann) was likewise intended for the solution of the differential equations, those describing the trajectory of projectiles above the Earth. And it is by no coincidence that it is the same class of problems that had led to the development of Calculus in the 17th century (Galileo, Huygens, Newton, Leibniz).
Two resulting communities — the analog and the digital — remained pretty much separated for a number of years, with some of the protagonists talking of a "war" between the two (which it was not). The digital side did gradually take over with the increasing power and decreasing cost of its hardware. Little analog computation was left by the middle 1970's.
What is today at the center of IMACS's disciplinary interests may be described in broad terms as the development of theoretical concepts and algorithmic

tools that use computers (digital computers : analog computers have become practically obsolete) and mathematics, in the abstract as well as in the context of specific applications. They are "tools" in the sense that they will -at least in theory- be used by others, members of some "end-use discipline" such as engineering and physics.

Those directions have changed and will by definition continue to change with time. New groups with particular interests appear, old ones become dormant although some have shown remarkably stubborn resilience to do so irrespectively of what was happening in the outside world. We have in our midst nice examples and counter-examples of the dynamics of what Thomas Kuhn called "Scientific Revolutions".

Working groups and technical committees

New disciplinary groups appear in IMACS generally manifesting themselves at first by a few individuals having the intent of organizing a workshop or conference, then asking for or being offered our sponsorship -something that gives them recognition, status and the possibility of having the outcome of their work published in established journals .

Working groups after a while often become organized and administered as Technical Committees – IMACS TC's – which consist of individual members that generally belong to academia. What is possibly the most important role of IMACS's in this process is in recognizing new fields of research, establishing contact with representative members of those emergent communities. The connection with those groups works is often started at first informally – at the professional instead of administrative level (between professors, established researchers, etc. …). It has been with the establishment and coordination of such connections that IMACS has been changed from an association with very little happening between the Triennial World Congresses (which is what it was up to the 1970's) and what it is now (we have about 13 "Technical Committees" in IMACS – generating jointly about one IMACS sponsored conference a month somewhere in the world).

The journals

Since 1979 IMACS bylaw states that the association publishes a scientific journal, Mathematics and Computers in Simulation, besides an information bulletin, IMACS Newsletter, for promoting scientific activities, launching conferences and workshops conceived by the affiliated research groups.

Recently the collaboration of IMACS with Elsevier has been enriched with the inclusion also of the journal Applied Numerical Mathematics as a further reputable editorial site for submitting interesting results for publication and for the publication of Special Issues with the best papers from IMACS events.

(from the official website of IMACS https://www.imacs-online.eu)

About *IMACS2023*

This booklet contains all the abstracts of the results which are going to be presented at the IMACS World Congress taking place in Rome at the Engineering Faculty of University 'La Sapienza', September 11-15, 2023.
This is the 21st one in a series of World Conferences whose complete list goes back to 1955 and covered the whole continents as it reads:

1955 Brussels, Belgium
1958 Strasbourg, France
1961 Opatija, Yugoslavia
1964 Brighton, Great Britain
1967 Lausanne, Switzerland
1970 Munich, Germany
1973 Prague, Czechoslovakia
1976 Delft, The Netherlands
1979 Sorrento, Italy
1982 Montreal, Canada
1985 Oslo, Norway
1988 Paris, France
1991 Dublin, Ireland
1994 Atlanta, USA
1997 Berlin, Germany
2000 Lausanne, Switzerland
2005 Paris, France
2009 Cairns, Australia
2013 Madrid Spain
2016 Xiamen, China

The subsequent World Conferences, usually, take place every three years. Unfortunately, due to the COVID pandemics, IMACS2023, initially scheduled in 2020, had to be postponed also in order to follow the spirit of the IMACS World Conference which prescribes to gather scientists in presence from all over the world. So, in the present occasion, the whole participants are expected to convene in Rome for exchanging their works, ideas and experiences.
This Book of Abstracts, reflecting the Congress structure, is organized in sections: Keynote Lectures, General Session, Mini-symposia, Special Sessions and Posters. According to the IMACS philosophy, different aspects of applied mathematics are represented with a special interest towards the numerical methods and solutions.

IMACS2023 FOREWORD

This is the *Book of Abstracts* for the **IMACS 2023** Congress. This meeting, as the long series of the IMACS World Congresses, aims at giving the opportunity to a large number of researchers and scientists to meet, facing each other in Rome, and discuss scientific computing results and future trends to support strong multidisciplinary communities. The Congress attendees have the opportunity to compare ideas and match points of view, contributing to the IMACS knowledge community combining expertise in the area of simulation as well as in classical and new applications.

The world is changing fast, and research communities face a range of new problems, not only those traditionally linked to the hard sciences and industry, but also those attached to the social sciences, to the impact of climate change, urban pollution, crowd dynamics, transportation and so on.

In line with the general philosophy of IMACS, this Congress opens the mind on different aspects of multidisciplinary problems coming from the real world as well as from the development of new theoretical and computational tools. Representatives of several research Institutions join in the Congress General Sessions, and in Mini-symposia and Sessions organized by separate Committees, showing advanced research developments in crucial application areas. Special Issues of the IMACS Journals, APNUM and MATCOM, will be published.

The publication of this Book of Abstracts, volume 23 in the IMACS Series in Computational and Applied Mathematics, which is edited by the members of the Local Organizing and Scientific Committee, Sandra Carillo, Costanza Conti, Daniela Mansutti, Francesca Pitolli and Rosa Maria Spitaleri, presents the large international participation in the 21st IMACS World Congress, organized by the *International Association for Mathematics and Computers in Simulation* (*IMACS*) with the sponsorship of the *Istituto per le Applicazioni del Calcolo* (*IAC*) of the Consiglio Nazionale delle Ricerche (CNR), along with the *University of Rome La Sapienza* and *University of Florence*.

Special thanks are due to the Congress Organizers, in particular the IMACS President, Dr. Rosa Maria Spitaleri, Chair of IMACS 2023 for her generous efforts, being the main contributor to the success of this event. Further thanks are due to all the Organizing Committees, Congress Staff and all the Participants.

Robert Vichnevetsky

IMACS Honorary President

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POSTERS 320

KEYNOTE LECTURES

Approximation of Non Linear Hyperbolic Problems and Property of Conservation

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In this talk, I am interested in problems of the type

$$\frac{\partial u}{\partial t} + \text{ div } f(u) = 0 \tag{1}$$

written on Ω an open subset of $\mathbb{R}^d$. The solution u belongs to $D \subset \mathbb{R}^p$, and the flux is $f = (f_1, \ldots, f_d)$ where the f_i are smooth functions defined on D with values in $\mathbb{R}^p$. This problem is equipped with initial conditions and boundary conditions, and is assumed to be hyperbolic, i.e. for any $\mathbf{n} = (n_1, \ldots, n_d)$, the matrix

$$\sum_{i=1}^{d} \frac{\partial f_i}{\partial x_i} n_i$$

is diagonalisable on $\mathbb{R}$. The typical example is that of the Euler equations.

Since the celebrated theorem by Lax and Wendroff who showed that a numerical scheme for (1) written in conservation form, if it is stable, will converge to a weak solution of the approximated hyperbolic problem, most of the work in this area of Research has been focussed on schemes that can be written, in a way or another, with flux. This is obviously true for finite volume schemes, whatever the order of accuracy, this is also true for a class of scheme using the discontinuous Galerkin paradigm: they use a discretised version of the weak form, and numerical flux.

However, there exist many schemes that seems no to be in a flux form. An example is the streamline diffusion method, and more generally continuous stabilized finite element methods. And it is also known they work very well !

In this talk, I show that all the known schemes, except maybe one (the so-called Active Flux scheme by Roe and co-authors), can be reformulated in flux form thanks to a reformulation of the conservation property. I will show how to exploit this reformulation to construct schemes compatible with other conservation constraints, such as the entropy inequality, and more generally speaking thermodynamical compatibility, or schemes on staggered grids.

Arbitrarily High Order Finite Element Methods for Arbitrarily Shaped Domains with Automatic Mesh Generation

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Partial different equations with discontinuous coefficients having complex interface geometry are of great interests in practical applications. The design of body-fitted high-order finite element methods requires the construction of shape regular body-fitted meshes for complex geometry and also nonlinear element transforms from the reference element to the elements with curved boundary. In practical applications, it may be challenging to satisfy the conditions imposed on the nonlinear element transforms in the literature which depend on the geometry of the interface.

In this talk we study high-order unfitted finite element methods on Cartesian meshes with hanging nodes for elliptic interface problems, which release the work of body-fitted mesh generation and provide a natural way to design high-order methods without resorting to nonlinear element transforms. We introduce new concepts of large element and interface deviation to solve the small cut cell problem of unfitted finite element methods. We construct a reliable algorithm to merge small interface elements with their surrounding elements to automatically generate the finite element mesh whose elements are large with respect to both domains. We show novel *hp*-domain inverse estimates which allow us to prove the stability of the finite element method under practical interface resolving mesh conditions and prove *hp* a priori and a posteriori error estimates. We propose new basis functions for the interface elements to control the growth of the condition number of the stiffness matrix in terms of the finite element approximation order, the number of elements of the mesh, and the interface deviation. Numerical examples are presented to illustrate the competitive performance of the method.

This talk is based on joint works with Ke Li, Yong Liu and Xueshuang Xiang.

Forecasting Damage and Consolidation: Mathematical Models of Reacting Flows in Monumental Stones

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In the last few years some mathematical models have been introduced to assess the evolution of damage due to atmospherical agents on natural stones used in monuments and historical artifacts. Besides, these models can be modified to take into account also the effect of some consolidation procedures, using different chemical compounds. In this talk I will present some of these models, which are based on a physico-chemical description in terms of partial differential equations, and their agreement with experimental data.

Mathematical Modeling of Oncological Data: A Multiscale Perspective

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This talk will describe a computational approach to the mathematical modeling of oncological data recorded at different scales by different experimental modalities. A specific focus will be devoted to the many aspects concerned with the use of inverse problems methods for the numerical reduction of these models. Applications will involve the use of hybrid imaging methods for the assessment of leukemic patients, the investigation of glucose metabolism in cancer tissues and the simulation of a specific transition in cancer cells by means of molecular interaction maps.

Patterns in Turbulent Convection: the Evergreen Rayleigh-Benard Problem

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Rayleigh-Bénard (RB) convection has been intensively studied since more than one hundred years, both experimentally and theoretically and, more recently, numerically. A testbed for ideas in nonlinear dynamics, chaos theory, turbulence, coherent structures and pattern formation, this simple idealized setup has become the *Drosophila* of nonlinear fluid dynamics and it is still a source of surprises and new phenomena. Here, I review a series of (mainly numerical) recent and semi-recent results on RB convection at moderate values of the Rayleigh number, up to Ra=10^8, focusing on the effects of plume clustering, internal cooling, Prandtl number variation and tilted rotation. A final discussion concerns the application of RB convection to the ice-capped ocean of the Jovian satellite Ganymede. The results presented here involved many colleagues and students who will be properly mentioned. This work is dedicated to the memory of our colleague, friend and master, Edward A Spiegel.

Rise and Fall of Popularity on Social Media

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We introduce a novel kinetic model of opinion formation on social networks, which takes into account a realistic statistical description of the background connectivity of the users [1, 2]. Then we propose to couple the model with a kinetic description of the spreading of the popularity of online content (such as e.g., advertisements, texts, videos and the like) based on the interactions of such content with the evolving opinions of the users. Analytical investigations and numerical simulations show that the coupled model can explain the emergence of time trends such as the rise and fall of popularity of hashtags empirically observed in real social media campaigns. The model also provides insights into communication strategies which may be better suited to foster the permeation of messages in the society.

References

[1] N. Loy, M. Raviola, A. Tosin. Opinion polarization in social networks, Philos. Trans. Roy. Soc. A, 380(2224):20210158/1-15, 2022.

[2] G. Toscani, A. Tosin, M. Zanella. Opinion modeling on social media and marketing aspects, Phys. Rev. E, 98(2):022315/1-15, 2018.

Modeling Traffic Jam and Growth Process of Neurons Using IGA and PGNN

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The motor-driven intracellular transport plays a crucial role in supporting a neuron cell's survival and function. The disruption of transport may lead to the onset of neurodegenerative diseases. To study how neurons regulate the material transport process, we develop a PDE-constrained optimization model and an isogeometric analysis (IGA) solver [1] to simulate traffic jams induced by microtubule reduction and swirl. We also develop a novel IGA-based physics-informed graph neural network (PGNN) [2] to quickly predict transport phenomena in neurons, which contains two simulators (pipe and bifurcation) and a GNN assembly model. The well-trained model effectively predicts the distribution of transport velocity and material concentration during traffic jam and normal transport with an average error <10% compared to IGA simulations. As a follow up, we propose a new phase field model with isogeometric collocation [3] to simulate multi-stages of neuron growth by considering the effect of tubulin, including lamellipodia formation, initial neurite outgrowth, axon differentiation, and dendrite formation. By incorporating experimental neurite features, we generate similar morphologies at multi-stages with formation of neurite networks. A CNN model is built to efficiently predict the growth process.

References

[1] A. Li, Y. J. Zhang, *Modeling Intracellular Transport and Traffic Jam in 3D Neurons Using PDE-Constrained Optimization*, Journal of Mechanics, 38:44-59, 2022.

[2] A. Li, Y. J. Zhang, *Isogeometric Analysis-Based Physics-Informed Graph Neural Network for Studying Traffic Jam in Neurons*, Computer Methods in Applied Mechanics and Engineering, 403:115757, 2023.

[3] K. Qian, A. Pawar, A. Liao, C. Anitescu, V. Webster-Wood, A. Feinberg, T. Rabczuk, Y. J. Zhang, *Modeling Neuron Growth Using Isogeometric Collocation Based Phase Field Method*, Scientific Reports, 12:8120, 2022.

GUEST LECTURE

Research Integrity & Publishing Ethics: A Whistlestop Tour of Common Ethical Pitfalls by Well-intentioned Researchers

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Unethical research can undermine trust in an author's research, their institute, the journal, a field of science, scholarly publishing and in science generally. Elsevier has an ongoing mission to safeguard research integrity in publishing by (1) providing editors the best tools, processes and policies, and (2) giving readers information required to assess the trustworthiness of published papers. In this session, Elsevier's Research Integrity & Publishing Ethics Centre of Expertise will present a whistlestop tour of common ethical pitfalls by well-intentioned researchers. By attending, you will gain insights on the following topics: Ethical consents & declarations, Authorship rights, Generative AI policies, Falsification, fabrication, and plagiarism, and Predatory journals & paper mills.

GENERAL SESSION

Numerical Approximations for Some Fractional Stochastic Partial Differential Equations-cases of Nonlinear Heat and Burgers Equations

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In this work, we interest in the study of the numerical approximations for some fractional stochastic partial differential equations in the Hilbert space $L^2(0,1)$; perturbed by a Gaussian noise and driven by the fractional Laplacian. Precisely, we use the implicit Euler scheme and the spectral Galerkin method, to approximate the mild solutions of; the fractional stochastic nonlinear heat equation (FSNHE) in time and in space and the fractional stochastic Burgers equation (FSBE) in time. Moreover, we make a combination of the of Galerkin and Euler methods to obtain the full approximation of the FSNHE. We calculate the rates of convergence of all those schemes and show their dependence on the fractional power of the Laplacian.

An Analysis of Boundary Perturbations in Laplace-Steklov Eigenvalue Problems

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In this study, we consider Laplace-Steklov eigenvalue problems defined in a way that the spectral parameter is involved in both the differential equation and the boundary conditions. Our primary concern is in the alteration of the spectrum of the associated operator resulting from a number of perturbations on the domain boundary. In order to analyze this influence, we derive Hadamard type formulas for both simple and multiple eigenvalues of the operator. These are employed to obtain the rate of change of the eigenvalues of the problem as its domain changes, which are not available in the literature to the best of our knowledge. As a consequence, we investigate, both analytically and numerically, the convergence behaviors of the eigenvalues for the problems defined on discs and regular polygons. The numerical simulations are carried out by using a finite element method with continuous Lagrange elements.

Analysing the Well-posedness of Networked first-order Hyperbolic Systems of Fluid Flow

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First-order hyperbolic systems are used to model different phenomena such as gas flow, shallow water flow, blood flow in arteries and veins, as well as multi-phase flow. Such flow can be complicated due to the fact that in interesting nonlinear cases the requisite solutions of Riemann problems may be discontinuous and weak solutions are considered. To identify physically relevant solutions, an entropy condition is employed. In this paper, these ideas are extended to flows in a networked domain. In such domains different simple domains are coupled at nodes of the network. At nodes half-Riemann problems are solved and well-posedness is proved. A presentation of the numerical approaches with appropriate boundary conditions at the nodes or vertices of the network will be made. Numerical examples are presented to demonstrate the approximate solutions that are obtained. A discussion of the numerical results will be made and appropriate conclusions and open questions will be presented.

Deep Image Prior Based Segmentation for Noisy Images

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In digital image processing and analysis a very challenging task is the segmentation of noisy images. Over the past few decades, one popular technique to tackle this task relies on the minimization of the Mumford-Shah (MS) energy and its approximations as the Ambrosio-Tortorelli (AT) one [1]. Recently, deep learning has led to a new generation of high-performing image segmentation models. In this work we expand the unsupervised deep learning approach [2] based on the Deep Image Prior (DIP) model [3] where both the MS and the AT functionals are parameterized by the weights of a convolutional neural network. The DIP model's implicit regularization allows to work with noisy input images and it appears robust with respect to both different noise levels and different types of noise. The proposed approach provides promising results on both biomedical and natural images.

References

[1] L. Ambrosio et al., *Approximation of functional depending on jumps by elliptic functional via t-convergence*, Comm. Pure Appl. Math., 1990.

[2] A. Benfenati et al., *Piece-wise Constant Image Segmentation with a Deep Image Prior Approach*, International Conference on Scale Space and Variational Methods in Computer Vision, 2023.

[3] D. Ulyanov et al., *Deep Image Prior*, Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition, 2018.

Response Function for Linearized Saint-Venant Equations with Uniformly Distributed Lateral Inflow

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In this work, we find the discharge corresponding to linearized full Saint-Venant equations by considering uniformly distributed lateral inflow along the channel length for a finite-length rectangular channel. The discharge due to the lateral inflow is presented as the convolution of two functions: lateral inflow distributed along the channel and lateral channel response function. We study the behaviour of the lateral channel response function for different cases of reference discharge, channel width, Manning roughness coefficient, and bottom slope. This function gets affected by the upstream and downstream boundary conditions. For a given channel width, the choice of reference discharge and slope of the channel plays a crucial role in the accuracy of the hydrograph. The meaning of semi-infinite channels also seems to vary with the slope of the channel. We observe that the downstream boundary condition cannot always be ignored, and for these cases, we observe its influence on the hydrographs plotted upstream. The results tally well with those of Mormarco et al. [1] and Cimoreli et al. [2, 3] and in fact, they cover certain issues not addressed earlier.

References

[1] T. Moramoarco, Y. Fan, R. L. Brass *Analytical solution for channel routing with uniform lateral inflow*, Journal of Hydraulic Engineering, 125, 707-713, 1999.

[2] L. Cimorelli, L. Cozzolino, R. Dela Morte *Analytical solutions of the linearized parabolic wave accounting for downstream boundary condition and uniform lateral inflows*, Advances in Water Resources, 63, 57-76, 2014.

[3] L. Cimorelli, L. Cozzolino, A. D'Aniello *Exact solution of the Linear Parabolic Approximation for flow-depth based diffusive flow routing*, Journal of Hydrology, 563, 620-632, 2018.

Simulating How Climate Change Affects Cultural Heritage Deterioration

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Cultural Heritage (such as Monuments, Historical and Modern Buildings, Archaeological sites) exposed to environment are subjected to decay. Such a decay can be caused by numerous factors, such as weathering, chemical aggression, or abrasion. In case of stone artifacts, deterioration and damaging might be caused by the water flowing into the porous matrix by groundwater rise or rain falling. Chemical substances dissolved in water penetrate within stones and react with it modifying the original structure and composition. Carbonation is one of the main decaying process of cultural heritage: it is caused by the chemical reaction of Carbon Dioxide dissolved in water with the consequent weakening of the porous matrix.
Since the atmospheric concentration of Carbon Dioxide has continuously increased in the last centuries, it is reasonable to think that carbonation effects might intensify. In order to assess the degradation of Building Heritage in a changing Climate, we present a mathematical model describing transport of water and chemical substances as well as the chemical reactions leading to concrete carbonation processes. After we calibrated the model with experimental data (found in literature), we simulate the degradation processes under different Carbon Dioxide concentration scenarios in atmosphere from IPCC reports (https://www.ipcc.ch/).
The study here presented is focused on concrete, since it is the most widely used construction material worldwide as it is employed in the construction of buildings, stadiums, stairs, sidewalks, foundations. Our results describe how the position of the carbonation front and the porosity change of the cement matrix under different Carbon Dioxide Scenarios.

Numerical Solutions of the Velocity–Vorticity Formulation of the Navier–Stokes Equations by Using the Localized Ghost Point Method

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In this study, a meshless numerical scheme, based on the localized ghost point method (LGPM), is proposed to accurately and efficiently solve the velocity-vorticity formulation of the Navier-Stokes equations. The Navier-Stokes equations, which represent the conservation laws of mass and momentum, are the governing equations for the flow fields of viscous incompressible fluid. In order to avoid dealing with the troublesome boundary condition of pressure, the velocity-vorticity formulation of the Navier-Stokes equations can be derived by introducing the definition of vorticity. Since the velocity-vorticity formulation of the Navier-Stokes equations are a system of time-dependent nonlinear partial differential equations, a suitable numerical scheme is required to obtain the flow fields of viscous incompressible fluid. The proposed meshless numerical scheme is the combination of the LGPM, which is responsible for spatial discretization, the fully implicit Euler method, which is used for temporal discretization, and the Newton-Raphson method, which is adopted for solving the system of nonlinear algebraic equations at every time step. The LGPM, truly free from mesh generation and numerical quadrature, is formed by combining the ghost point method and the concept of localization. Comparing with the conventional localized radial basis function collocation method, the LGPM outperforms in terms of accuracy by distributing the ghost points within an extended domain. Furthermore, the fully implicit Euler method can ensure the stability for temporal discretization, as the Newton-Raphson method will maintain the efficiency for solving nonlinear systems. As a result, the proposed meshless numerical scheme can provide excellent accuracy, stability and efficiency for numerical simulations. Several numerical examples are presented in this study to verify the merits of the meshless numerical scheme in this study.

Steady-state Density Preserving Method for Second-order Stochastic Differential Equations

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We devise a method for the long-time integration of a class of damped second-order stochastic systems. The introduced numerical scheme has the advantage of being completely explicit for general nonlinear systems while, in contrast with other commonly used integrators, is able to compute the evolution of the system with high numerical stability and precision in very large time intervals. Notably, the method has the important property of preserving, for all values of the step-size, the steady-state probability density function of any linear system with a stationary distribution. Numerical simulations are presented to illustrate the practical performance of the introduced method.

References

[1] de la Cruz, H, *Steady-state density preserving method for stochastic mechanical systems*, Eur. Phys. J. Plus, 136, 799, 2021.

[2] de la Cruz, H, *Stabilized explicit methods for the approximation of stochastic systems driven by small additive noises*, Chaos, Solitons & Fractals 140, 2020.

Surface Effects on Propagation of Shear Horizontal Waves on Nonlocal PE-PM Bilayer Structure with an Imperfect Interface

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This study investigates the nonlocal and surface effects on the dispersion properties of Shear horizontal (SH) waves in piezoelectric- piezomagnetic bilayer structure with an imperfect interface. Nonlocal Magnetoelectroelastic(MEE) theory is used to derive the general governing equations by introducing an intrinsic length. Surface effects exerting on the boundary conditions of the PE-PM bilayer structure are taken into account through the incorporation of the surface piezoelectricity and surface piezomagnetism model and the generalized Younge-Laplace equations. The closed form of the dispersion equation has been obtained analytically for electrically open and magnetically short surface conditions. Numerical solutions were utilized to investigate the effects of nonlocal scale parameters and surface parameters on the size-dependent characteristics of dispersion behaviors on SH surface wave propagation. It has been observed that the thickness of the bilayer has a significant effect on the phase velocity of the wave. Also, It has been noted that mechanical imperfect parameter between the interface of PE and PM bilayer structure impacts the phase velocity. The results can be found helpful for the development and production of smart composite structures.

References

[1] Eringen AC, Edelen DGB, *On nonlocal elasticity*, Int J Eng Sci, 1972.

[2] Gurtin, Morton E., and A. Ian Murdoch, *Surface stress in solids*, International journal of Solids and Structures, 1978.

[3] Zhang, L.L., Liu, J.X., Fang, X.Q. and Nie, G.Q., *Effects of surface piezoelectricity and nonlocal scale on wave propagation in piezoelectric nanoplates*, European Journal of Mechanics-A/Solids, 2014.

Numerical Simulation of 3D Vorticity Dynamics with the Diffused Vortex Hydrodynamics Method

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Three-dimensional free vorticity dynamics is simulated with a new 3D version of the Diffused Vortex Hydrodynamics (DVH) method. Similarly to the corresponding 2D approach, the 3D variant of DVH is characterized by the use of a regular distribution of points, or "lattice", to perform the diffusion of the vorticity field and by a suitable choice of diffusion and advection time steps.

The diffusion step is performed through the superposition of elementary heat equation solutions over a cubic support of $N_d \times N_d \times N_d$ lattice points (where N_d ranges by 4 to 8 depending on the set accuracy level). This redistribution during the diffusion step avoids excessive clustering or rarefaction of the vortex particles providing robustness and high accuracy of the method.

The meshless interaction between vortices is carried out through a Barnes-Hut tree code implemented in the general-purpose algorithm PEPC (Pretty Efficient Parallel Coulomb-solver), which is an open-source tree code that was developed at Jülich Supercomputing Centre since the early 2000s (DOI 10.5281/zenodo.7965548).

Convergence tests on two benchmarks of free vorticity are discussed, where results from literature are considered as a comparison: the first is the classic evolution of a vortex ring at $Re_\Gamma = 500$, whereas the second is a side-by-side collision of two vortex rings at $Re_\Gamma = 1153$. Conserved quantities as linear impulse and total vorticity are checked during time integration.

The simulations are aimed at the evaluation of the best trade-off between accuracy and calculation speed.

Numerical Solutions of Three-dimensional Elliptic Partial Differential Equations by the Method of Fundamental Solution and the Particle Swarm Optimization

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In this study, a meshless numerical scheme, which is the combination of the method of fundamental solutions (MFS) and the particle swarm optimization (PSO), is proposed to accurately and efficiently analyze three-dimensional boundary value problems, governed by elliptic partial differential equations. The MFS is a well-known boundary-type meshless methods, since it is truly free from mesh generation and numerical quadrature. Although the MFS can acquire extremely accurate solution via a very simple numerical procedure of collocation, it is known that the spatial locations of sources in the MFS may have great influence on the numerical accuracy of the MFS. In the study, we adopted the PSO to determine the optimal spatial locations of sources in the MFS so as to efficiently obtain highly-accurate solutions of three-dimensional elliptic partial differential equations. The PSO, which is one of the newly-developed metaheuristic algorithms, can optimize a problem by iteratively improving the candidate solutions. In this research, several three-dimensional numerical examples, governed by elliptic partial differential equations, will be provided to verify the effectiveness of the PSO and validate the performance of the proposed MFS-PSO. In addition, the discussions of potential engineering applications by using the proposed MFS-PSO will be demonstrated in this presentation.

Radial Basis Function Interpolation for Child's Hand X-ray Image Processing

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Radial basis functions (RBFs) are mathematical functions that depend on the distance from center points and are commonly used in interpolation, approximation, numerical simulation, and machine learning applications [1]. RBFs are characterized by their ability to take on different shapes, such as Gaussian or cubic, and to be symmetrical around the center point. RBFs are often used to model complex, nonlinear relationships between input and output data and are particularly useful when dealing with high-dimensional data. They have been applied in various fields, including finance, engineering, and natural language processing. Typically they are applied in topography approximation [2].

This study uses the RBFs interpolation for the child's hand X-ray image processing. These images are used in medicine for bone age assessment. It is a medical technique used to estimate a child's age by examining their bones development. The assessment involves comparing the person's bone development with a standardized reference atlas to determine if it is consistent with their chronological age or is delayed or advanced [3]. Typically, the assessment is based on the child's left-hand X-ray image. The method is commonly used to evaluate children's growth disorders or hormonal imbalances. The study applies the RBFs interpolation for background estimation and image registration of the child's left-hand images. The presented examples are based on publicly available datasets. The advantages and disadvantages are also discussed.

References

[1] M.D. Buhmann, *Radial Basis Functions: Theory and Implementations*, Cambridge University Press, 2003.

[2] R.L. Hardy, Multiquadric Equations of Topography and Other Irregular Surfaces, *J. Geophys. Res.*, Vol. 76(8), 1971, pp. 1905-1915.

[3] V. Gilsanz, O. Ratib, *Hand Bone Age. A Digital Atlas of Skeletal Maturity*, Springer, 2012.

Improved Growth Estimate of Infinite Time Blowup Solution for a Semilinear Hyperbolic Equation with Logarithmic Nonlinearity

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In this topic, we discuss an improved estimate of the infinite time blowup solution for the semilinear wave equation with logarithmic nonlinearity. Comparing the previous work, this improved growth estimate not only provides the information about the relationship between the power of the nonlinearity and the growth, but also gives a faster growth estimate. The proof of the main conclusions is carried out at the negative initial energy level, the sub-critical initial energy level, the critical initial energy level and the arbitrary positive initial energy level.

The Qualitative Behavior for One-dimensional Sixth-order Boussinesq Equation with Logarithmic Nonlinearity

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The Cauchy problem for the nonlinear one-dimensional sixth-order Boussinesq equation with logarithmic nonlinearity is concerned in this paper. This model describes the propagation of long waves on the surface of water within small amplitude. The main motivation of this paper is to reveal how logarithmic nonlinearity $u\ln|u|^k$ along with the higher-order dispersive term u_{xxxxxx} affects the qualitative properties of the solution. Some of the efforts on results of global existence and exponential growth of the solution are shown. The main tools to obtain these results include the logarithmic Sobolev inequality, Galerkin method and the concave method. The initial energy is divided into different cases by the depth of the potential well, and corresponding results for subcritical and critical energy levels are both given.

On Some Oscillatory Properties of Finite Difference Methods for One-Dimensional Nonlinear Parabolic Problems

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It was shown in [1] that, under some relatively simple conditions, the number of the local maximizers and minimizers of the solution of one-dimensional nonlinear parabolic problems does not grow in time. In this talk we consider the finite difference solutions of the problems and give conditions that guarantee the discrete analogue of the above property. The conditions yield some bounds that restrict the choice of the spatial mesh size and the time step. We use the theory of totally nonnegative matrices [2] in the derivation of the bounds. The results are demonstrated with numerical examples.

References

[1] K. Nickel, Gestaltaussagen über Lösungen parabolischer Differentialgleichungen, Journal für die reine und angewandte Mathematik, 211, 78–94, 1962.

[2] S. M. Fallat, C. R. Johnson, Totally Nonnegative Matrices, Princeton Series in Applied Mathematics, 2011.

Optimal Upgrade Policy Model for Used Product Leased with Lemon Law

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In this paper, we present an upgrade cost model for a used product protected by lemon laws during a lease period. The product is declared a lemon if either of two conditions are met: (i) the product has been returned to the lessor k times (e.g., k=4) to have the failed product fixed, or (ii) the product has been out of service more than the pre-specified threshold (e.g., 30 days) due to one or more failures. The optimal upgrade policy is determined to minimize the lessor's total expected servicing cost which is the sum of upgrade cost and lemon servicing cost during the lease period. Furthermore, two options are presented: (i) refund and (ii) replacement. Both options are optimized upgrade policies for used products, which allow the lessee choose the most suitable lease contracts among the available options offered by the lessor. Numerical examples are provided to demonstrate the proposed models. This study provides the lessor of used products with useful guidelines on designing flexible and optimized lease contracts.

Equation-Oriented Process Simulation: The Simultaneous Flash

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This contribution continues the line of results [1] demonstrating power of rigorous mathematical approach combined with modern simulation technology in solving simulation and optimization problems of chemical engineering.

The Equation Oriented (EO) modeling architecture is effective alternative to the Sequential Modular modeling approach proved to be useful for complex plants and effective for executing advanced simulation scenarios, calibration of model parameters, data reconciliation, and, most important, process optimization. Phase equilibrium is fundamental to the process modeling. The EO modeling has strict requirements to the fundamental modeling layer, the Simultaneous Flash framework. Classical thermodynamic equilibrium problem (termed as the Flash in process industry) requires global minimization of the thermodynamic criterion. Because of its optimization nature, the Flash problem cannot be expressed in terms of equations only (the latter is still not well understood in academia and industry). We have implemented the approach based on rigorous mathematical conditions written in the form that allows effective EO formulation. The Simultaneous Flash ensures the thermodynamic validity of the EO simulation results. Key feature of the Simultaneous Flash is support for flexible model structure, the critical functionality that enables large scale process simulation and optimization. The thermodynamic model automatically adapts to the state conditions. The latter ensures the convergence and numerical efficiency. We discuss the Simultaneous Flash in the context of the Unisim Design process simulator.

References

[1] M. Lazman, *Algebraic Problems of Thermodynamics* 17th IMACS World Congress Scientific Computation, Applied Mathematics and Simulation, Paris, France, July 11-15, 2005, CD ROM ISBN: 2915913021, 9782915913026, Paper–T2

Localized Nonsingular Method of Fundamental Solutions for Two-dimensional Laplace Problems

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This work aims to develop further a Localized Nonsingular Method of Fundamental Solutions (LNMFS) for solving two-dimensional Laplace problems. The LNMFS removes the artificial boundary for each local subdomain present in the Localized Method of Fundamental Solutions (LMFS). The singularities are substituted by the normalized area integrals of the Fundamental Solution (FS) over small squares, covering the source points that intersect with the collocation points. The respective desingularized values of the derivatives of the FS, as required in Neumann boundary conditions, are calculated indirectly by considering a reference solution of the Laplace equation. The feasibility and accuracy of the newly developed method are demonstrated through comparison with analytical solutions for several Laplace problems. The advantage of the new approach is removing the necessity to search the position of the artificial boundary for each subdomain.

Application of a Haar Wavelet Based Numerical Method to a Moving Obstacle Avoidance Problem for Unmanned Aerial Vehicles

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Application of optimal control problems can be found everywhere, including science laboratories, industries, and day-to-day life. For example, in a room, the task of maintaining a given temperature in the quickest time via control of airflow from the air conditioner, minimizing the cost of energy in path planning of a mobile robot together with avoiding obstacles static or dynamic, minimizing cost of fuel in the driving of an autonomous car, minimizing of time in the flying of a drone from one point to another point, minimizing time in launching a missile and hitting the target static or dynamic, landing of a spacecraft on the moon with minimum energy, minimizing the cost in control of infectious diseases like dengue, malaria, COVID-19, etc. It is quite a common scenario that we may not be able to analytically solve the given nonlinear optimal control problem in the presence of nonlinear constraints with the available methods. Therefore, we need to look for numerical methods which can give at least approximate solutions to the considered optimal control problem with any given accuracy we desire. In this work, we present an application of Galerkin's Haar wavelet-based numerical method to solve a minimum time/energy optimal control problem for an unmanned aerial vehicle and avoid a static/moving obstacle in its path when planning to start from a given point to a destination point. It converts the given nonlinear control problem into a nonlinear optimization problem. On solving it, we obtain an approximate solution of the state as well as the control variable together with the cost. We further show the error in the state, control variables as well as in cost values for different numbers of Haar wavelets basis functions. This shows the convergence of the numerical scheme as well as accuracy.

Surface Effect on Lamb Wave Propagation in a Nonlocal Piezo-Electric and Piezo-Magnetic Bi-Material Plate

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In this article, the impact of surface elasticity and nonlocal small-scale effects on lamb wave propagation in a bi-material plate consisting of piezoelectric and piezo-magnetic materials has been investigated. The nonlocal electroelasticity theory is employed to obtain the general governing equations by introducing an intrinsic length. By including the surface piezoelectricity model and Young-Laplace equations, the surface effects acting on the boundary conditions of the electro-magnetic nanoplates are taken into account. The dispersion relations obtained in matrix form by employing electro-magnetic boundary conditions In numerical results, it can be shown that both the nonlocal parameter and surface piezoelectricity have a significant influence on the wave dispersive behavior.

Solution of Fuzzy-fractional Allen-Cahn Equations Using a Robust Numerical Approach

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This article considers nonlinear time-fractional-fuzzy Allen-Cahn equations [1] that represent the oil pollution in the water. The fuzzy-fractional Allen-Cahn equations are solved approximatively using a generalised Newton polynomial interpolation method [1] and compared with the homotopy analysis generalised transform method [2] to check the efficiency of the proposed method. The diffusion coefficient D has been taken as a Gaussian fuzzy number to comprehend the nature of the Allen-Cahn equation in an uncertain situation. Finally, numerical and graphical data validate the results with the exact solution.

References

[1] Akinfe TK, Loyinmi AC. An improved differential transform scheme implementation on the generalised Allen-Cahn equation governing oil pollution dynamics in oceanography. Partial Differential Equations in Applied Mathematics, 2022, 6.

[2] Atangana A, Araz SI. New numerical scheme with Newton polynomial: theory, methods, and applications. Academic Press; 2021.

[3] Sartanpara PP, Meher R. Solution of generalised fuzzy fractional Kaup–Kupershmidt equation using a robust multi parametric approach and a novel transform. Mathematics and Computers in Simulation. 2023; 205:939-69.

Development of Almost Unbiased Modified Ratio Estimators for Population Mean Using Unknown Population Parameter(s)

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This paper discusses the estimation of the population mean of the study variable when the information on the auxiliary variable is unknown and their population parameters are unknown. In times past, a number of modified ratio estimators were suggested with known values of population parameters such as the coefficient of variation. Coefficient of kurtosis, coefficient of skewness, population correlation coefficient etc. The above mentioned estimators are biased with minimum mean squared error compared to classical ratio estimator. However, the auxiliary variable is not available in all cases. In this paper, double sampling design was applied to obtain the information on the auxiliary variable and their population parameters, which were used to construct almost unbiased modified ratio estimators. These estimators were subjected to a linear cost function to determine whether the reduction in variance worth the extra cost required to observe the auxiliary variable. The almost unbiased modified ratio estimators performed better the modified ratio estimators. These are explained with the help of numerical examples.

Impact of Nonlocal Piezoelectricity on Propagation of Torsional Wave in Piezoelectric Fiber-Reinforced Composite

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This study investigates the impact of nonlocality on the propagation of torsional waves in piezoelectric fiber-reinforced composites (PFRC) layer on top of a functionally graded elastic substrate. The PFRC is assumed to be composed of piezoelectric fiber and an epoxy matrix. The analysis begins by considering the constitutive relations for piezoelectric materials and incorporating the effects of nonlocality. Nonlocality accounts for the long-range interactions and the influence of neighboring points on the deformation response. The governing equations for torsional wave propagation, considering the coupled electromechanical behavior of the piezoelectric constituents, are derived, taking into account the nonlocal effects. A theoretical derivation based on the nonlocal theory of the PFRC model is carried out and the dispersion relation for the torsional wave has been derived under non-classical mechanical and electrical boundary conditions. Through numerical simulations and analytical techniques, the impact of nonlocality on the dispersion, phase velocity of torsional waves in piezoelectric fiber-reinforced composites is examined. The results reveal that nonlocal effects significantly affect the propagation characteristics of torsional waves. The nonlocal behavior introduces additional modes, alters the dispersion behavior, and affects the phase velocity. This study provides valuable insights into the complex wave dynamics, helping to optimize the performance and functionality of such composites in various engineering applications.

References

[1] Eringen AC, Edelen DGB, *On nonlocal elasticity*, Int J Eng Sci, 1972.

[2] Kumar, Anil, and D. Chakraborty, *Effective properties of thermo-electro-mechanically coupled piezoelectric fiber reinforced composites*, Meccanica, 2009.

[3] Dhua, Sudarshan, and Chattopadhyay, Amares, *Torsional wave in an initially stressed layer lying between two inhomogeneous media*, Meccanica, 2015.

Multi-Agent Reinforcement Learning for Strategic Bidding in Two Stage Electricity Markets

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Our goal is to study the dynamics of electricity markets involving multiple competitive generators through multi-agent reinforcement learning (MARL) approaches. We start by formulating the electricity market as a two-stage stochastic game, involving a finite set of conventional and renewable energy producers, which bid on the day-ahead market, and an Independent System Operator (ISO), which is responsible for the clearing of the market. We assume that a predetermined part of the producers are non-strategic, bidding at their marginal costs, while the others might bid strategically trying to learn the outcome of the clearing. In the first stage, the strategic producers optimize simultaneously their bids by minimizing their expected costs (opposite of the expected profits), which is the difference between their production cost and the payment they receive from the ISO. The renewable energy producers' objective functions include a penalty assigning a cost to the imbalances caused by their forecast errors. In the second stage, the ISO receives the bids of all the producers. It clears the market by determining the activated volumes for each producer and a price minimizing the total cost under capacity constraints, including a conditional value at risk (CVaR) constraint for the renewable producers, capturing the risk aversion level that the requested volume violates their uncertain capacity. We derive closed form expressions for the producers' best-responses considering payas- clear and pay-as-bid as pricing schemes, and simulate the market dynamics, using MARL. To that purpose, we rely on modified versions of two actor-critic algorithms: Deep Deterministic Policy Gradient and Soft Actor-Critic. The simulations show how the producers adapt dynamically their strategies to learn the best bidding strategy, under limited information exchange. Finally, we identify conditions for the convergence of MARL algorithms to local equilibria of the stochastic game.

A Deep Neural Network Discontinous Galerkin method for solving PDEs involving discontinuities

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We consider Deep Neural Networks (NNs) for solving Partial Differential Equations (PDEs) with possibly discontinuous solutions. To do so, we first partition the domain into elements, and introduce a NN architecture that has as an input the element number and intends to approximate the solution at the mesh-nodes of each given element. Then, we introduce a quadratic loss function composed of the Ritz energy functional plus certain jumps in the solution and inter-element fluxes to weakly impose continuity/discontinuity conditions. Finally, we train the NN using exact (Gaussian) integration and differentiation techniques under the assumption that the solution inside each element is given by a polynomial of a given degree (typically, one or two). The resulting method is combined with a recently developed r-adaptive method for NNs [1] that allows to optimize the mesh via proper movements of the mesh nodes.

In the presentation, we will describe the proposed Deep Discontinuous Galerkin method (DDGM) and demonstrate its effectiveness through numerical results applied to test problems in one and two spatial dimensions.

References

[1] Omella, Á.J., Pardo, D. $r-$Adaptive Deep Learning Method for Solving Partial Differential Equations. arXiv preprint arXiv:2210.10900. (2022).

Multi-objective Optimization of the Appendages of a Sailing Yacht Using the Normal Boundary Intersection Method

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The underwater part of a sailing yacht is equipped with a couple of wings (*appendages*). The simplest configuration consists of only two appendages: the keel fin and the rudder, each subject to different flow conditions. The keel fin, whose main role is to counteract the lateral forces generated by the wind, cannot change its orientation, and it has a small incidence with respect to the flow. Instead, the rudder, that generates the forces moving the yacht from one course to another, can rotate around a vertical axis, and it can experience large angles of attack with respect to the local flow, with the risk of separation of the flow and a sudden loss of performance. Consequently, two different designs are required, considering also a range of flow conditions for both. We have two different multi-objective optimization problems, where the final solution is not unique, and a trade-off between the different optimal solutions is required. The optimization algorithm must provide a rich and precise determination of the so-called *Pareto front*, in order to have a large set of alternatives.

Different single-objective optimization algorithms have been adapted for the solution of a multi-objective problem. The Normal Boundary Intersection method (NBI) [1], conversely, has been designed specifically for the solution of this class of problems: it searches directly the Pareto front, gaining information from the objective function space and not from the design variable space. In this paper, a variant of NBI [2], including also other techniques for the direct search of the Pareto front, will be described and applied. The different options provided by the algorithm will be further analyzed.

References

[1] I. Das and J.E. Dennis, *Normal-boundary intersection: A new method for generating the Pareto surface in nonlinear multicriteria optimization problems.* SIAM Journal of Optimization, 8(3):631–657, 1998.

[2] D. Peri, *Direct Tracking of the Pareto Front of a Multi-Objective Optimization Problem*, J. Mar. Sci. Eng. 2020, 8(9), 699; https://doi.org/10.3390/jmse8090699

Numerical Study of Non-linear Time Fractional Model of HIV/AIDS Transmission

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HIV/AIDS is a serious medical disease that decreases the immune system of the human body, leaving the sufferer vulnerable to neurological diseases, uncommon cancers, and life-threatening infections. HIV/AIDS is a serious disease that is transmissible. The transmission of HIV/AIDS among humans is examined using a nonlinear temporal fractional epidemic system model. Here we use the alternative numerical scheme called fractional Adams–Bashforth scheme. The technique produces an effective numerical methodology for using fractional order derivative. The obtained numerical results are illustrated using graphs that show how the population of susceptible, HIV-infected (with/without AIDS symptoms), and HIV-infected on antiretroviral treatment changes over time. Also, the comparative analysis of obtained numerical results with other method is given for validation.

References

[1] Gao, W., Günerhan, H. and Baskonus, H.M., 2020. Analytical and approximate solutions of an epidemic system of HIV/AIDS transmission. Alexandria Engineering Journal, 59(5), pp.3197-3211.

[2] Toufik, M. and Atangana, A., 2017. New numerical approximation of fractional derivative with non-local and non-singular kernel: application to chaotic models. The european physical journal plus, 132, pp.1-16.

An Algebraic Technique for Determining the Maximal Cliques in a Graph

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The computational problem of determining maximal cliques of a graph has connections to many real-world applications.

Finding maximal cliques is important in terms of graph coloring. For instance, the size of a largest maximal clique of a chordal graph equals the chromatic number of the graph. Determining maximal cliques is a non-deterministic algorithm. Some well known algorithms like Karp's 21 NP-complete problem, Brute-force search, Bron-Kerbosch algorithm, and others are time consuming and hard problems in dealing with graphs containing large number of vertices. Although simpler algorithms like perfect elimination ordering for finding a maximal clique of a chordal graph is available, the problem is NP-hard for general graphs.

The graph operations like union, intersection and join can be transformed to algebraic operations satisfying certain axioms and a graph can be described by an algebraic expression. The method has been used by a number of authors to study graph structures.

Let $\mathcal{S}_n$ be the set of all simple graphs whose vertex set is contained in $\{v_1, \ldots, v_n\}$. Then, the union (denoted by $+$) and the join (denoted by $\cdot$) are binary operations on $\mathcal{S}_n$. Considering a vertex v as the graph containing the single vertex v , we show that every graph in $\mathcal{S}_n$ can be expressed uniquely as an algebraic expression in a normal form in variables $v_1, \cdots, v_n$, i.e., as a sum of a minimal number of monomials. Each of the monomials in the normal form then corresponds to a maximal clique in the graph.

We provide an algorithm to obtain the normal form from the given adjacency relations defining the graph, and thereby all maximal cliques in the graph.

High Order Compact ADI Scheme for two Dimensional Non-linear Reaction Subdiffusion Equation

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This study aims to devise an efficient numerical method for solving a 2-dimensional non-linear time fractional reaction subdiffusion equation of order $\alpha \in (0,\ 1)$. The time fractional derivative in the model problem is approximated using the $L2-1\sigma$ scheme, and space derivatives are approximated using a compact finite difference scheme. Computational cost is reduced using Newton's linearized method and alternating direction implicit method. The solvability, stability, and convergence analysis of the discussed scheme are studied rigorously. The applicability of the discussed numerical scheme is established by illustrative examples.

A Meshless Approach for Generalized Finite Difference Schemes

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This work presents a novel meshless Generalized Finite Difference (GFD) approach to solve partial differential equations on irregular regions. The proposed method eliminates the need for a regular grid structure, making it well-suited for problems where the domain is non-convex or non-simply connected. The effectiveness of this approach is shown through numerical experiments on a range of test problems, including stress and deformation, heat transfer, advective, and advective-diffusive problems. The results show that the proposed meshless GFD approach outperforms the traditional GFD method regarding accuracy and computational efficiency, especially for problems with complex geometries. Overall, this new approach provides a flexible and robust framework for solving PDEs and has the potential to be applied to several applications in various fields of engineering and science, such as the ones to be presented in this work.

Mathematical Models on Brain Networks for the Progression of AD

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Alzheimer's disease (AD) is the most common form of dementia. It is well-known that two proteins, namely beta amyloid and altered forms of tau protein, have a key role in neurodegenerative processes. The mechanisms linking the widespread and progressive deposition of these toxic proteins to the progression of the disease are only partially understood and are subject of active ongoing investigation. In addition, recent studies point out that beta amyloid and tau protein act in a synergetic fashion amplifying each others toxic effects.
The aim of this talk is to present different mathematical approaches to the modeling of toxic proteins' spreading throughout the brain in AD by means of reaction-diffusion equations on a finite graph, whose vertices represent functionally homogeneous brain regions and whose edges describe the connections between such regions. In the first part of the talk, a novel approach to model transport phenomena of toxic tau protein along the edges of the brain network will be presented, whose key idea consists in determining the mass transfer of toxic tau at each time between the nodes of the network by means of the steady-states solution of a suitable system of PDEs (firstly developed in [1]) defined on the edges. Some numerical simulations will be shown which demonstrate the effectiveness of this approach in capturing key features of the AD progression in the brain. The second part of the talk is dedicated to the analysis of a model based on finite-dimensional Smoluchowski-type system for the dynamics of both toxic beta-amyloid and tau proteins, where the mass transfer of the toxic proteins is described by means of the graph laplacian. The main mathematical and computational novelty is the introduction of two superposed graphs: in addition to the neural network, where the intracellular tau protein diffuses, a second graph is needed to model the spread of the extracellular beta-amyloid protein. Some numerical simulations will be discussed, where various modeling hypothesis have been tested to explore the impact of the interaction and the synergetic action of the two protein types in the progression of Alzheimer's disease.
The results presented in this talk are part of joint works and ongoing collaboration with M. Bertsch (U. Roma 2), A. Raj and J. Torok (UCSF), B.Franchi, M.C. Tesi (U. Bologna).

References

[1] J. Torok, P D. Maia, P. Verma, C. Mezias, A. Raj Emergence of directional bias in tau deposition from axonal transport dynamics. *PLoS Comput Biol* 17(7): e1009258, 2021.

On a Solow Model with Spatial Diffusion and Technology-induced Motility

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This work studies a parabolic-ODE PDE's system which describes the evolution of the physical capital "k" and technological progress "A", using a meshless in one and two dimensional bounded domain with regular boundary. The well-known Solow model is extended by considering the spatial diffusion of the capital accumulation. Moreover, we study the case in which spatial movement of k towards the higher concentrations of A, the technology progress. For such models, we propound schemes based on the Generalized Finite Difference method and proof the convergence of the numerical solution to the continuous one. Several examples show the dynamics of the model for a wide range of parameters. These examples illustrate the accuary of the numerical method.

References

[1] Benito J. J., García A., Gavete L., Negreanu M., Ureña F., Vargas A. M. *Solving a fully parabolic chemotaxis system with periodic asymptotic behavior using generalized finite difference method.*Applied Numerical Mathematics 157, 356-371.

[2] Capasso V., Engbers R., La Torre D., *On a spatial Solow model with technological diffusion and nonconcave production function.* Nonlinear Analysis: Real World Applications 11 (2010) 3858–3876.

[3] Solow R., A contribution to the theory of economic growth, Quarterly Journal of Economics 70 (1956) 65-94.

Global Existence and Blow up of Solutions for Pseudo-parabolic Equation with Singular Potential

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In this talk, we like to report a study in the initial boundary value problem of pseudo-parabolic equation with singular potential, in order to classify the initial data for the global existence, finite time blowup and longtime decay of the solution. The whole study is conducted by considering three cases according to initial energy: low initial energy case, critical initial energy case and high initial energy case. For the low initial energy case and critical initial energy case the sufficient initial conditions of global existence, long time decay and finite time blowup are given to show a sharp-like condition. Also two different strategies are applied to estimate the upper bounds of the blowup time for the negative initial energy blowup and positve initial energy blowup respectively. And for the high initial energy case, the finite time blowup is proved.

Numerical Method for Solving System of Cauchy Singular Integral Equations of Index Zero

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Cauchy singular integral equations and their systems frequently occur in the field of crack problems in fracture mechanics, water scattering problems in hydrodynamics, the flow around thin airfoils in aerodynamics, neutron transport, etc. There is no general method to find an analytical solution to these problems. Therefore, numerical methods have been developed to obtain their approximate solutions as closely as possible, which includes collocation methods, quadrature methods, Nystrom method, etc. But the search for a better numerical method in terms of easy implementation, better rate of convergence, better error bounds, etc., is always there. For this purpose, we develop a Chebyshev polynomial-based residual method for solving the system of Cauchy singular integral equation of index zero. Index zero implies that there is a singularity in the solution at one end of the bounded interval [-1,1], and it should be handled with great care in assuming the form of the approximate solution. Further, the singular integral in the Cauchy singular integral equations does not exist in the Riemann sense and must be interpreted with respect to the definition of the sense of Cauchy principal value. We first show that the given system of Cauchy singular integral equations is well-posed in the sense of Hadamard. We further derive the error estimates for the proposed numerical scheme. We also show that the numerical scheme is well-posed. We investigate the rate of convergence of the proposed numerical scheme. We show an illustration of the proposed numerical method through examples. We will make a comparison of our obtained results with the results present in the literature.

Global Well-Posedness for a Class of Semilinear Hyperbolic Equations with Singular Potentials on Manifolds with Conical Singularities

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This paper is concerned with a class of semilinear hyperbolic equations with singular potential on the manifolds with conical singularities, which was introduced to describe a field propagating on the spacetime of a true string. We prove the local existence and uniqueness of the solution by using the contraction mapping principle. In the spirit of variational principle and mountain pass theorem, a class of initial data are precisely divided into three different energy levels. The main ingredient of this paper is to conduct a comprehensive and systematic study on the dynamic behaviour of the solution with three different energy levels. We introduce a family of potential wells to derive a threshold of the existence of global solutions and blow up in finite time of solution in both cases with subcritical and critical initial energy. Moreover, two sets of sufficient conditions for initial data leading to blow up result are established at arbitrarily positive initial energy level.

MINI-SYMPOSIA

MS1 - ADAPTED TIME-INTEGRATORS FOR DIFFERENTIAL AND INTEGRAL PROBLEMS WITH APPLICATIONS

Organizers:

Angelamaria Cardone, Dajana Conte, Severiano Gonzalez Pinto, Beatrice Paternoster

The aim of this Mini-Symposium is to gather researchers working on the numerical solution of evolutionary problems that model different types of natural phenomena and physical processes, by means of differential or integral equations, also with stochastic perturbations. Particular attention will be dedicated to the time-integration through problem-oriented and efficient numerical methods, which are able to accurately follow the qualitative and quantitative behaviour of the solution, possibly also using parallel computation strategies. Applications in different contexts will be considered, among which: environmental models, material corrosion, porous media, plasma physics, image restoration, population and epidemic models, information diffusion models, wave propagation models, network dynamics, call option pricing in finance.

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Numerical Issues Arising in the Equation for the Unsaturated Flow in Porous Media

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We present some issues related to the numerical solution of the Richards' equation, which describes water flow in unsaturated porous media: we first consider discontinuities in space occurring when representing flow in layered soils, and we propose a transversal method of lines able to recast our problem in a Filippov framework. We treat both a 1D and 2D spatial domain case, with tailored numerical schemes (for more details, see [1, 2]).
Afterwards, in a irrigation framework, we introduce discontinuities in the root water uptake functions, and we propose a simplified optimal control approach for maximizing root water uptake while at the same time minimizing the amount of water provided for irrigation, as in [3].

References

[1] M. Berardi, F. V. Difonzo, M. Vurro, L. Lopez, *The 1D Richards' equation in two layered soils: a Filippov approach to treat discontinuities*, Advances in Water Resources, 115 (2018), pp. 264–272.

[2] M. Berardi, F. V. Difonzo, L. Lopez,, *A mixed MoL–TMoL for the numerical solution of the 2D Richards' equation in layered soils*, Computers & Mathematics with Applications, 79(7) (2020), pp. 1990–2001.

[3] M. Berardi, M. D'Abbicco, G. Girardi, M. Vurro, *Optimizing Water Consumption in Richards' Equation Framework with Step-Wise Root Water Uptake: A Simplified Model*, Transport in Porous Media, 141 (2022), pp. 469-–498

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Accurate Simulation of the NLS Equations via Multiple-Relaxation ImEx Methods

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The nonlinear Schrödinger equation possesses an infinite hierarchy of conserved densities, making the numerical preservation of some of these quantities critical for accurate long-time simulations, particularly for multi-soliton solutions. In this talk, I will present an essentially explicit discretization in time by combining higher-order Implicit-Explicit (ImEx) time integrators with multiple relaxation and adaptive step size control, ensuring the conservation of the first two quantities using a conservative finite element spatial discretization. I will demonstrate the effectiveness of our proposed method and compare it with the popular time-splitting pseudo-spectral approach that uses operator splitting in time and pseudo-spectral spatial approximation in space. Our results show that the proposed method performs well in accurately simulating nonlinear Schrödinger equations in the semiclassical regime and outperforms other existing methods in the presence of multi-soliton solutions.

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The Class of Implicit-explicit General Linear Methods for Ordinary Differential Equations

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The class of implicit-explicit (IMEX) methods are numerical scheme designed for numerical solution of ordinary differential systems with splitting of the right hand sides of the differential systems into two parts, one of which is non-stiff or mildly stiff, and suitable for explicit time integration, and the other part is stiff, and suitable for implicit time integration.

We described the construction of IMEX general linear methods with desired stability properties. Under suitable assumptions such as the form of coefficient matrices, order and stage order of methods, the form of stability function we attempt to maximize the combined region of absolute stability. Finally, we apply constructed methods to a series of test problems.

This is a joint work with A. Cardone, Z. Jackiewicz and P. Pierzchała.

References

[1] M. Braś, A. Cardone, Z. Jackiewicz, P. Pierzchała, *Error propagation for implicit-explicit general linear methods*, Appl. Numer. Math., 131 (2018), pp. 207–231.

[2] A. Cardone, Z. Jackiewicz, A. Sandu, H. Zhang, *Extrapolation-based implicit–explicit general linear methods*, Numer. Algorithms, 65 (2014), pp. 377—399.

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An Efficient Gauss-Newton Method for Non-linear Inverse Problems via Generalized Krylov Subspaces

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The solution of nonlinear inverse problems is a challenging task in numerical analysis. In most cases, this kind of problems are solved by iterative procedures that, at each iteration, linearize the problem in a neighborhood of the currently available approximation of the solution. The linearized problem is then solved by a direct or iterative method. Among this class of solution methods, the Gauss-Newton method is one of the most popular ones. We propose an efficient implementation of this method for large-scale problems. Our implementation is based on projecting the nonlinear problem into a sequence of nested subspaces, referred to as Generalized Krylov Subspaces (GKS), whose dimension increases with the number of iterations, except for when restarts are carried out. When the computation of the Jacobian matrix is expensive, we combine our iterative method with secant (Broyden) updates to further reduce the computational cost. We show convergence of the proposed solution methods and provide a few numerical examples that illustrate the performance of the proposed methods.

References

[1] A. Buccini, P. Díaz de Alba, F. Pes, and L. Reichel, *An efficient implementation of the Gauss-Newton method via generalized Krylov subspaces*. Submitted, 2023.

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Exponential Integrators for Problems with d-Dimensional Kronecker Structure

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In this talk, we consider efficient ways to approximate actions of the exponential and of φ-functions for matrices A with a d-dimensional Kronecker sum structure, that is $A = A_d \oplus \cdots \oplus A_1$. This is of paramount importance when applying exponential integrators to certain evolutionary partial differential equations semidiscretized in space.

The key point is the evaluation of the action of the matrix exponential $\exp(A)$ by using a concatenation of μ-mode products (the so-called Tucker operator), realized by high performance level 3 BLAS. The whole procedure involves just exponentials of the *small sized* matrices A_μ, and does not require forming the *large sized* matrix A. This technique already guarantees speedups of several order of magnitude in some exponential integrators of Lawson or splitting type.

The approach is then extended to φ-functions, by applying Gaussian quadrature formulas to their integral representation combined with a scaling and squaring technique. In addition, it allows for the computation of linear combinations of actions of φ-functions, which is of particular interest for high order exponential integrators. Finally, a direction splitting for approximating actions of φ-functions in well-established exponential integrators is introduced. The desired actions are realized again in a μ-mode fashion by using few Tucker operators. Several numerical experiments with 3D semidiscretized partial differential equations show consistent speedups with respect to state-of-the-art techniques to approximate (linear combinations of) actions of φ-functions.

References

[1] M. Caliari and F. Cassini. Direction splitting of φ-functions in exponential integrators for d-dimensional problems in Kronecker form arXiv:2304.02327 [math.NA], 2023.

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A Class of Nystrom Type Methods for the Numerical Integration of Second Order Differential Equations

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Explicit Runge-Kutta-Nyström (RKN) methods for the numerical solution of inhomogeneous linear initial value problems with constant coefficients are considered.

A general procedure to construct explicit s-stage RKN methods with maximal order $p = s + 1$, similar to the developped by the authors [1] for the class of second order IVP under consideration, depending on the nodes $c_i, i = 1, \ldots, s$ is presented. This procedure only requires the solution of succcessive linear equations in the elements a_{ij}, $1 \leq j < i \leq s$ of the matrix of coefficients $\mathbf{A}$ of the explicit RKN method and avoids the solution of non linear equations.

The remarkable fact is that using as free parameters the nodes $c_i, i = 1, \ldots, s$ with a quadrature relation, the $s(s-1)/2$ a_{ij} elements of matrix $\mathbf{A}$ can be computed by solving succesively linear systems with coefficientes depending on the nodes, so that if they are non-singular we get a unique s-stage methods with maxmal order $s + 1$.

We obtain an optimized six-stage seventh-order RKN method in the sense that the nodes are chosen so that minimize the leading term of the local error. Finally, some numerical experiments are presented to test the behaviour of the optimized RKN method with others RKN ones.

References

[1] Montijano, J. I.; Rández, L.; Calvo, M.; Explicit Runge-Kutta methods for the numerical solution of linear inhomogeneous IVPs. J. Comput. Appl. Math. 425 (2023))

Modified Singly-RKTASE methods for the solution of stiff problem

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In a recent paper, Calvo and coworkers (Journal of Scientific Computing, 2023) proposed a new class of TASE operators that improve previous TASE operators (Bassene et al., J. Compu. Phys.,2021 and Calvo et al. Journal of Scientific computing, 2023) in the sense that instead of involving the inverse of several different matrices, they have only a unique matrix inverse. This can improve greatly the efficiency if LU factorization is used to solve the associated linear systems. A disadvantage that Runge-Kutta TASE methods have compared to other one step methods for the solution of stiff systems, such as Rosenbrock or W methods, is that the coefficients of their leading local error is large, and this reduces their practical efficiency. In this talk we present a modification of singly TASE operators that gives more free parameters that can be used to reduce the error coefficient. Moreover, using the equivalence between W methods and RK-TASE methods given by S. González-Pinto and coworkers (to appear in Appl. Numer. Math.) it is possible to reduce the order of the TASE operator yet maintaining the order of the Resulting RK-TASE scehme, and this allows to obtain methods with smaller error coefficients. Some numerical experiments show the performance of the new schemes

References

[1] M. Bassenne, L. Fu, and A. Mani. Time-Accurate and highly-Stable Explicit operators for stiff differential equations. Journal of Computational Physics 424 (2021): 109847.

[2] M. Calvo, J.I. Montijano, L. Rández. A note on the stability of time-accurate and highly-stable explicit operators for stiff differential equations. Journal of Computational Physics 436 (2021): 110316.

[3] M. Calvo, L. Fu, J. I. Montijano and L. Rández. Singly TASE operators for the numerical solution of stiff differential equations by explicit Runge-Kutta schemes. Journal of Scientific computing (2023)

[4] S. González-Pinto, D. Hernández-Abreu, G. Pagano, S. Pérez-Rodríguez. Generalized TASE-RK methods for stiff problems. To appear in Applied Numerical Mathematics

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A Magnus Integrator for Stochastic Oscillators

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In this talk, we propose a numerical method for solving second order scalar stochastic differential equations of the form

$$\ddot{x} = (h(t)x + f(t, x(t)))dt + \varepsilon\xi(t) \tag{2}$$

where $f : [0, T] \times \mathbb{R}$ and $\xi(t)$ is a white noise process satisfying $\mathbb{E}|\xi(t)\xi(t')| = \delta(t - t')$. Equation (2) describes a class of nonlinear oscillators with non-constant frequency. The proposed scheme extends the idea of Magnus integrators to the stochastic case and its convergence properties are here rigorously analyzed. Selected numerical experiments on relevant stochastic oscillators confirm the effectiveness and the competitive behaviour of the method, with respect to standard integrators.

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Numerical Conservation Issues for Stochastic PDEs

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In this talk, we address our attention to the numerical solution of the stochastic Korteweg-de Vries equation [3]. The exact flow of such stochastic partial differential equation satisfies invariant laws [4]. In particular, the averaged spatial integral of the first moment of the solution is constant in time while the spatial integral of the second moment of the exact flow grows, in average, linearly in time. Here, we aim to analyze such characterizing properties exhibited by the exact solution also along suitable numerical approximations given by a central finite difference scheme for the spatial discretization [5] and by stochastic ϑ-methods for time integration [2]. The investigation has revealed that such invariant laws are not retained along the aforementioned approximations; indeed, we prove that linear and quadratic terms (in time) appear, destroying the eventual conservative character of such discretizations [1]. Selected numerical experiments have also been provided to confirm the theoretical results.

References

[1] R. D'Ambrosio, S. Di Giovacchino, *Numerical conservation issues for the stochastic Korteweg-de Vries equation*, J. Comp. Appl. Math. 424, 114967 (2023).

[2] D. Higham, *Mean-square and asymptotic stability of the stochastic theta method*, SIAM J. Numer. Anal. 38, 753–769 (2000).

[3] D.J. Korteweg, G. de Vries, *On the change of form of long waves advancing in a rectangular canal, and on a new type of long stationary waves*, Philos. Mag.. 39, 422–443 (1895).

[4] G. Lin, L. Grinberg, G.E. Karniadakis, *Numerical studies of the Stochastic Korteweg-de Vries equation*, J. Comput. Phys. 231 (2), 676–703 (2006).

[5] A.C. Vliegenthart, *On Finite-Difference Methods for the Korteweg-de Vries Equation*, J. Eng. Math. 5 (2), 137–155 (1971).

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Numerical and Parallel Issues for Cellular Behavior Prediction

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Cell behavior research plays a pivotal role in formulating treatments for diseases and has implications in embryonic development, tissue regeneration, and cancer progression. Mathematical models like agent-based models (ABMs), reaction-diffusion models (RDMs), and lattice-based models (LBMs) have been devised to understand biological processes through cell evolution modeling. These models integrate parameters like cell adhesion and deformability for simulating activities such as cell migration and tissue morphogenesis, with LBMs being notably computationally efficient. The Cellular Potts Model (CPM) [1], grounded on energy minimization principles, is an exemplary model. Various enhancements to CPM capture aspects like spatial heterogeneity and chemotaxis, enhancing its predictive abilities for intricate biological systems. Nevertheless, some CPM implementations lack the finite element method (FEM), which escalates computational complexity. To address this, a parallel GPU implementation of CPM, incorporating FEM for energy system evaluation, has been proposed. Utilizing modern GPUs and the CUDA programming model, this implementation efficiently simulates and analyzes cellular behavior, thus maximizing parallel processing and boosting simulation efficiency.

References

[1] Glazier, J. A., & Graner, F. (1993). Simulation of the differential adhesion driven rearrangement of biological cells. Physical Review E, 47(3), 2128.

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Efficient Numerical Methods for High-dimensional Itô Stochastic Differential Equations

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We are concerned with the efficient computation of weak approximations to the solutions of high-dimensional Itô stochastic differential equations (SDEs). In [2], by providing a linear error analysis and utilizing a Strang splitting-type approach, we have derived explicit stochastic Runge–Kutta (RK) methods for high-dimensional Itô SDEs. The methods achieve weak order 2 and have high computational accuracy for relatively large time-step size. In this presentation, as competitors, we take stochastic exponential RK methods of weak order 2 [3] and some existing stabilized explicit methods [1], and carry out numerical experiments on a variety of linear and nonlinear problems to check the computational performance of the methods. We will show that our proposed techniques are very effective especially for high-dimensional problems.

References

[1] A. Abdulle, G. Vilmart, and K. C. Zygalakis. Weak second order explicit stabilized methods for stiff stochastic differential equations. *SIAM J. Sci. Comput.*, **35**(**4**):A1792–A1814, 2013.

[2] Y. Komori and K. Burrage. Split S-ROCK methods for high-dimensional stochastic differential equations. Submitted to a journal.

[3] Y. Komori, D. Cohen, and K. Burrage. Weak second order explicit exponential Runge–Kutta methods for stochastic differential equations. *SIAM J. Sci. Comput.*, **39**(**6**):A2857–A2878, 2017.

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Minisymposium
Adapted Time-integrators for Differential and Integral Problems with Applications

Boundary Corrections for Splitting Methods in the Time Integration of Multidmensional Parabolic Problems

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Boundary corrections for the time integration of splitting methods in multidimensional parabolic PDEs are considered. A brief review of some techniques proposed in the literature is made [1, 2, 4]. The main focus is put on methods of AMF-W-type, which allow an important reduction in the algebra cost for the multidimensional case, at the point that it turns out to be similar to the 1D case times the number of spatial dimensions. We follow a MoL approach and assume Dirichlet boundary conditions, in which case, the proposed spatial discretization considers the boundary values as unknowns and the time-integration is carried out with AMF-W-type methods with directional splitting [3]. The numerical results confirm that this way avoids the marked order reduction linked with time-dependent boundary conditions and splitting methods, which does not appear for time-independent boundary conditions or well it is quite less pronounced. Some intuitive ideas by explaining the mitigation in the order reduction are also presented.

References

[1] L. Einkemmer and A. Ostermann, Overcoming order reduction in diffusion reaction splitting. Part 1: Dirichlet boundary conditions. SIAM J. Sci. Comput., 37 (2015) A1577–A1592.

[2] W. Hundsdorfer and J. G. Verwer, Numerical solution of time-dependent advection diffusion reaction equations, Springer Ser. Comput. Math. 33, Springer, Berlin, 2003.

[3] S. González Pinto, E. Hairer, D. Hernández-Abreu, and S. Pérez-Rodríguez. AMF-type W-methods for parabolic problems with mixed derivatives, Siam J. Aci. Comput., 40, No. 5, pp. A2905–A2929, 2018.

[4] S. González Pinto, D. Hernández-Abreu, and S. Pérez Rodríguez, AMFR-W-methods for parabolic problems with mixed derivates. Applications to the Heston model, Journal of Computational and Applied Mathematics 387 (2021) 112518

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Space-time Parallel Solvers for the Solution of Parabolic Problems

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In a context of computer archictectures with increasing number of calculation cores, the numerical solution of evolutionary problems can benefit from parallelization both in time and in space. In the framework of time parallel time integrators, parareal is one of the most celebrated methods [1]. It is an iterative algorithm that considers two propagators: one of them, cheap and fast, that is applied sequentially and the other one, expensive and more accurate, that is applied in parallel. In this work, we propose to consider two classical time-splitting schemes as propagators in the parareal algorithm, namely, the fractionary Implicit Euler method and the Douglas-Rachford scheme. Moreover, its combination with suitable alternating direction or domain decomposition splittings permits us to parallelize the computations also in space without the need of performing additional iterations. We show stability and convergence properties for both methods, remarking the importance of choosing L-stable methods in order to obtain stable space-time parallel schemes with faster convergence, as suggested in [2]. Along with these theoretical results, we show some numerical experiments that illustrate the behaviour of the designed methods.

References

[1] J.L. Lions, Y. Maday, G. Turinici (2001). *Résolution d'EDP par un schéma en temps "pararéel"*. C. R. Acad. Sci. (1) - Math., 337(7), 661-668.

[2] G.A. Staff, E.M. Ronquist (2005). *Stability of the parareal algorithm.* In T.J. Barth et al., editors, *Domain Decomposition Methods in Science and Engineering.* Lect. Notes Comput. Sci. Eng., vol. 40. Springer, 449-456.

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Minisymposium:
Adapted time-integrators for differential and integral problems with applications

On the Stability of IMEX-theta Methods for Parabolic PDEs with Delay

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In this work, we will analyse the stability of the θ-method, applied to the delay differential equation (DDE) with constant delay:

$$y'(t) = f(t, y(t)) + g(t, y(t), y(t-\tau)).$$

If it is combined with lineal interpolation for the terms with delay, then it can be written as follows:

$$y_{n+1} = y_n + h(1-\theta)[f(t_n, y_n) + g(t_n, y_n, (1-u)y_{n-m} + u \cdot y_{n-m+1})]$$

$$+h\theta[f(t_{n+1}, y_{n+1}) + g(t_{n+1}, y_{n+1}, (1-u)y_{n-m+1} + u \cdot y_{n-m+2})],$$

taking $h = \tau/(m-u)$, with $m \in \mathrm{N}$, $\theta \in [0,1]$ and $u \in [0,1)$. This method is only first-order in general, except for $\theta = \dfrac{1}{2}$ when it is second-order.

In the scientific literature, the stability of these methods is usually studied by analyzing the scalar equation

$$y'(t) = \lambda y(t) + \mu y(t-\tau), \quad \lambda, \mu \in \mathrm{C}.$$

However, in this way we reduce the study of stability to systems of DDEs

$$y'(t) = Ay(t) + By(t-\tau),$$

when A and B are simultaneously diagonizable, and therefore after a transformation it is analysed through the analysis of d scalar problems.

However, we will follow a newer theory that has only been used for some problems without delay, showing that it can also be used in problems with delay . In this way we will be able to check the asymptotic behavior of the corresponding θ-method when applied to these DDEs where A is a symmetric positive definite matrix (for example coming from diffusion), but A and B do not need being simultaneously diagonalizable. This is a first step to analyze the stability for some particular nonlinear partial differential equations with delay.

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A Numerical Method for Time-fractional Sub-diffusion Problems

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The time-fractional diffusion equation has been found in many real-life processes, where anomalous diffusion occurs. Due to the fact that the analytical solution of the fractional diffusion equation is not usually known, effective numerical methods are vital when solving real world problems. In this presentation, we will explore how combining two techniques—the method of lines and collocation method—can yield a higher degree of accuracy than a two-way discretization approach. To demonstrate our findings we investigate the initial value problem

$$D_t^\alpha u(x,t) - p\frac{\partial^2 u(x,t)}{\partial x^2} + \nu(x)u(x,t) = f(x,t) \tag{3}$$

for $(x,t) \in Q = (0,L) \times (0,b]$ with

$$u(0,t) = \psi_0(t), \quad t \in (0,b], \tag{4}$$
$$u(L,t) = \psi_L(t), \quad t \in (0,b], \tag{5}$$
$$u(x,0) = \phi(x), \quad x \in [0,L]. \tag{6}$$

where $0 < \alpha < 1$, p is a positive constant (also called in literature the general diffusion coefficient), $\nu \geq 0$ and $\nu, f, \psi_0, \psi_L, \phi$ are continuous in their respective fields. The idea is first use the method of lines: create a uniform mesh on the space-interval $[0,L]$ and approximate the space derivative in (3) by the second order finite difference. We get a system of equations for the $y_i(t) \approx u(x_i,t)$, where x_i is the gridpoint in $[0,L]$ and t belongs to $[0,b]$.
We denote $z_i = D^\alpha y_i$ and use the collocation-based approach to approximate z_{iN} using the graded grid on the time-interval $[0,b]$ and Lagrange fundamental polynomials.
In the talk we describe the existence, uniqueness and regularity properties of the solution to problem, study the convergence and convergence order of our method and present some numerical examples.

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Application of Exponential Integrators for a Phase-Field Dendritic Crystal Growth Model

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Phase-field modeling of dendritic solidification results in a highly nonlinear partial differential equations (PDEs) system. After spatial discretization, due to a significant difference between the time scales of phase-field and temperature PDEs, a fully explicit time integration scheme commonly solves the phase-field equation, and an implicit scheme solves the temperature equation. However, the stability criterion of the phase-field equation severely restricts the maximum allowable time step and results in large scale computational problems. On the other hand, fully implicit schemes, like the Newton method, are not feasible in practice because of a high computational cost per time step.

Here we applied exponential time-differencing schemes to solve spatially discretized phase-field equations corresponding to pure element solidification. The Krylov subspace approach is used to compute the action of matrix functions, φ-functions, on a desired vector. We implemented a fourth-order scheme with an embedded third-order scheme to estimate the error and automatically control the time step size. Our results show that the proposed method can afford a time-step size up to two orders of magnitude larger than the classic explicit method while reaching the same level of temporal accuracy. Moreover, the computational performance of the suggested scheme was superior compared to the explicit approach.

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A New Method to Solve the 2D Schrodinger Equation

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We consider, for a given potential function $V(x, y)$, the numerical solution of the two-dimensional linear time-independent Schrödinger equation

$$-\nabla^2\psi(x, y) + V(x, y)\psi(x, y) = E\psi(x, y)\,,$$

on a bounded, sufficiently regular domain $\Omega \subset \mathbb{R}^2$ subject to homogeneous Dirichlet boundary conditions. The solutions consist of real eigenvalues E and corresponding eigenfunctions $\psi(x, y)$.

The method we propose here is based on two ideas. Firstly, we were inspired by Ixaru, who presented in [1] an adaptation of a well-known technique developed by Titchmarsh: in the x-direction the eigenfunction is expressed in well-chosen, yet y-dependent sets of basis functions. To be specific, the chosen basis functions are the eigenfunctions of one-dimensional Schrödinger equations $-\dfrac{d^2\varphi}{dx^2} + \bar{V}^{(k)}(x)\varphi = \lambda\varphi$, where $\bar{V}^{(k)}(x)$ is piecewisely dependent on y. Secondly, in [2] a simple, easy to implement method based upon high order finite difference approximations is proposed that is able to attain similar accuracies as the method in [1]. The combination of these two ideas, together with the improvements from [3] and the use of very efficient algorithms for solving the one-dimensional Schrödinger equations [4], leads to a new method.

References

[1] L. Gr. Ixaru (2010), New numerical method for the eigenvalue problem of the 2D Schrödinger equation, *Comput. Phys. Commun.* 181 (2010) 1738–1742.

[2] Z. Wang and H. Shao (2009), A new kind of discretization scheme for solving a two-dimensional time-independent Schrödinger equation, *Comput. Phys. Commun.* 180 (2009) 842–849.

[3] T. Baeyens and M. Van Daele, Improvements to the computation of eigenvalues and eigenfunctions of two-dimensional Schrödinger equations by constant perturbation based algorithms, *J. Comput. Appl. Math.* 412 (2022) 114292.

[4] T. Baeyens and M. Van Daele, The fast and accurate computation of eigenvalues and eigenfunctions of time-independent one-dimensional Schrödinger equations, *Comput. Phys. Commun.* 258 (2021) 107568.

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Fighting Agroecosystems Pests with Operations Research Tools

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In agriculture pests contribute to the decrease of harvests. Nowadays also the new phenomenon of alien species invasions due globalization worsens these effects.

Dynamical models can be formulated to analyse, simulate and ultimately understand these processes. When all the possible system's outcomes can be determined, it is often found that they are related to each other via bifurcations. Pictorially, the situation can be represented by a graph where the nodes are the final states of the system and the arcs are their links, in which a bifurcation parameter plays an essential role. It is therefore possible to move from a final regime to a next one by acting on this parameter. When a critical threshold is crossed, the dynamical equations attain a different configuration. However, action on the parameter involves a cost: in ecology for instance, a culling strategy could be devised to raise the mortality of a population that represents a nuisance. Bringing the current state of the system to a pest-free environment may require traveling in the graph through several nodes and possibly this may be associated with different paths. We will illustrate a stragegy to minimize the total effort to achieve the desired result and assess the corresponding way to travel in the graph. Examples of the algorithm behavior will be given based on actual field situations and hypothetical costs associated to the ecosystems parameters.

MS2 - LINEAR AND NONLINEAR MODELS IN APPLIED MATHEMATICS

Organizers: Sandra Carillo, Galina Filipuk, Federico Zullo

This session is devoted to recent results concerning applicative problems modelled via differential and/or integro-differential equations. Contemporary challenges raised by current advances in engineering, applied science and in- dustry involve mathematical models which are more and more sophisticated. Indeed, new materials, such as materials with memory, bio- materials or mate- rials in which micro or nano particles are injected to change their mechanical or thermal response to external actions. Viscoelastic, magneto-viscoelastic and thermo-viscoelastic bodies are only few examples of materials that are deserving a growing interest both under the theoretical as well as the applicative point of view. The session aims to bring together researchers who are all investigating linear and nonlinear models in applied mathematics under different viewpoints to, possibly, encourage their interaction to find new results and perspectives via the contamination among their different methodological approaches. Advances in theoretical problems concerning mathematical modelling in differential equa- tions along with results of current interest in applications are welcome.

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Minisymposium
Linear and Nonlinear Models in Applied Mathematics

Media with Inclusions with Imperfect Transmission and Interface Potential

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We consider composites where a hosting medium contains a periodic array of inclusions, with period ε. The inclusions are coated by a layer consisting of thin sublayers of two different materials (with thickness of the order $\varepsilon\eta$ and $\varepsilon\delta$, respectively); the second sublayer encloses the first one. This bilayered coating material is such that the external part has a low diffusivity in the orthogonal direction, while the internal one has high diffusivity along the tangential direction. On the interface separating the two sublayers we assume perfect transmission conditions. All the parameters ε, η and δ are supposed to be very small, but with different orders. In particular, we perform, for fixed ε, a two-step concentration procedure.

We first let δ go to zero, a case for which we appeal to known literature. This step of concentration replaces the internal layer with a smooth surface, where an imperfect contact condition prevails, together with a tangential Laplace equation for the heat potential having as a source the jump of the normal flux. Then, we let η go to zero, thereby performing the concentration of the model already obtained. This concentration procedure involves the appearance of new effects on the resulting interface between the hosting material and the inclusions, and a new surface heat potential. Though somehow similar problems, involving jumps in the solution and also in the flux, as well as Laplace-Beltrami operators, already appeared in the engineering literature in connection with composite materials, they are usually justified by numerical simulations and by asymptotic analysis. Here we provide a fully rigorous mathematical approach. Finally, we homogenize the concentrated model, which is far from being a standard task. For example, the usual local cell problems involved in the homogenization procedure are, in our case, highly non-standard, calling also for properly adapted functional settings.

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Minisymposium
Linear and Nonlinear Models in Applied Mathematics

Probabilistic Analysis and Simulation of a Class of Compartmental Models Via Random Linear Differential Equation Systems

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Coupled linear systems are ubiquitous in modern science and engineering, both in mathematical modeling and simplifying complex models. Furthermore, uncertainty quantification is crucial for the analysis and prediction of any kind of exhaustive real-world mathematical model. Because of these two facts, this contribution analyzes a class of compartmental models, sometimes termed continuous-time birth models, that can be formulated via a system of random first-order ordinary differential equations of the form:

$$\begin{cases} y_1'(t,\omega) &= -a_1(\omega)y_1(t,\omega) + g_1(t,\omega), \\ y_2'(t,\omega) &= -a_2(\omega)y_2(t,\omega) + a_1(\omega)y_1(t,\omega) + g_2(t,\omega), \\ &\vdots \\ y_n'(t,\omega) &= -a_n(\omega)y_n(t,\omega) + a_{n-1}(\omega)y_{n-1}(t,\omega) + g_n(t,\omega), \end{cases} \tag{7}$$

where $a_1(\omega), \ldots, a_n(\omega)$ are random variables with finite variance (formally belonging to the random Lebesgue space $\in \mathrm{L}_2(\Omega)$), defined on a complete probability space, $(\Omega, \mathcal{F}, \mathbb{P})$. The source terms $g_i(t,\omega)$ are assumed to be stochastic processes.

In this contribution, we will first take advantage of the random Laplace transform to obtain a pathwise weak solution $(y_1(t,\omega), \ldots, y_n(t,\omega))$ in a recursive way in different scenarios of practical interest that include when the forcing terms $g_i(t,\omega)$ are: (1) random variables; (2) delta Dirac impulsive distributions with a random intensity and (3) Wiener processes. In all these scenarios, we will obtain the so-called 1-Probability Density Function of the solution under very general hypotheses. To achieve this goal, we use two main probabilistic tools, namely, the Random Variable Transformation technique and the Liouville equation, respectively. Apart from showing some numerical experiments with different probabilistic distributions for model parameters, we will apply Inverse Uncertainty Quantification techniques to show how to apply the theoretical findings to model a problem with real-world data.

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Linear and Nonlinear Models in Applied Mathematics

Superconductivity vs. Nematicity: a Ginzburg-Landau approach

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In this talk, we will show a system of equations that models, into a Ginzburg Landau regime, the response of a superconducting nematic liquid crystal medium in the presence of an external magnetic field. Since the Helmholtz free energy for this regime, described in [1], we derive a coupled system of Ginzburg-Landau equations. Particularly, we will focus only on the strip case $[0, d] \times [0, +\infty)$, where we obtain the following system:

$$\begin{cases} A'' = f^2 A \\ \kappa_s^{-2} f'' = f\left(A^2 + f^2 - 1 + \widetilde{v}\widetilde{\beta} g^2\right) \\ \kappa_n^{-2} g'' = g\left(\dfrac{4\pi^2 \xi_n^2}{d^2} + g^2 - 1 + \dfrac{\widetilde{v}}{\widetilde{\beta}} f^2\right) \end{cases} \tag{8}$$

where $A(x)$ is the magnetic vector potential, f(x) and g(x) are the order parameters, superconducting and nematic respectively. We will focus on the interplay between both order parameters and on the existence of a Freéderickz threshold for the nematic parameter, in the sense of [2], and we analyze the relationship between both order parameters, especially for the competition case (see [3]). Equation (8) extends the well known model for the superconducting case.

References

[1] D.G. Barci, R.V.Clarim, N.L. Silva Junior, *Vortex and disclination structures in a nematic-superconductor state*, Phys. Rev. B 94, 184507 (2016).

[2] D. García Ovalle, J.P. Borgna, M.F De Leo, *Freédericksz transition on a phenomenological model for a nematic inhomogeneous superfluid in present of an electric field.* Physica D Nonlinear Phenomena, vol 414, 132705 (2020).

[3] M.F. De Leo, J.P. Borgna, D. García Ovalle, *Interplay between nematicity and superconductivity in a Ginzburg-Landau regime* Submitted (2023).

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Nonlinear Evolution Equations of Fifth Order: Some New and Old Results

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Fifth order nonlinear evolution equations are considered: they all are connected via Bäcklund transformations. The links, portrayed in a wide *Bäcklund Chart* [1] are here revisited. Specifically, the Caudrey-Dodd-Gibbon-Sawada-Kotera (CGDSK) equation

$$u_t = \left(u_{xxxx} + \frac{5}{2} u u_x + \frac{5}{12} u^3 \right)_x$$

is considered. It is connected via Bäcklund transformations to the Kaup-Kupershmidt equation:

$$v_t + \left(v_{xxxx} + 10 v v_{xx} + \frac{15}{2} v_x^2 + \frac{20}{3} v^3 \right)_x$$

The established links are reconsidered and, inspired by results obtained in the case of third order nonlinear evolution equations of *KdV type*, new results are presented. In addition, the two Bäcklund Chart which connect, in turn, fifth and third order soliton equations are compared.

Third order soliton equations admit non-Abelian counterparts: they are all connected via a non-Abelian Bäcklund Chart [2] Possible extensions to non-Abelian counter parts are currently under investigation [3].

References

[1] C. Rogers, S. Carillo, *On reciprocal properties of the Caudrey-Dodd-Gibbon and Kaup-Kupershmidt hierarchies*, Physica Scripta, **36**, 865–869, (1987)

[2] S. Carillo, M. Lo Schiavo, C. Schiebold, *Abelian versus non-Abelian Bäcklund Charts: some remarks*, Evolution Equations and Control Theory, **8** (1), 43–55, (2019).

[3] S. Carillo, C. Schiebold, *non-Abelian fifth order soliton equations*, in progress.

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Linear and Nonlinear Models in Applied Mathematics

A Molecular Dynamics Study of the Evolving Melt Front under Gravity

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During melting under gravity in the presence of a horizontal thermal gradient, buoyancy-driven convection in the liquid phase affects significantly the evolution of the liquid-solid interface. Due to the obvious engineering interest in understanding and controlling melting processes, fluid dynamicists and applied mathematicians have spent many efforts to model and simulate them numerically. Their endeavors concentrated in the twenty-five years period between the publication of the paper by Brent, Voller & Reid (1988) and that by Mansutti & Bucchignani (2011). The former—and most of the following ones—adopted a phase-field model (where the interface is blurred into a smooth transition zone), while the latter was based on a Stefan-like model with sharp interface. With suitably chosen values of many ad-hoc material and numerical parameters, all of the above simulations were able to attain some agreement with their common benchmark, the melt fronts obtained experimentally by Gau & Viskanta (1986) on a sample of gallium enclosed in a parallelepipedal box with one vertical wall heated. This left unresolved several fine issues, such as whether the elastic response of the solid phase plays a role in determining the shape of the liquid-solid interface.

Here, for the first time, we tackle this problem at the atomistic level with a molecular dynamics approach. The advantage we gain is that a unique microscopic model describes all of the aggregation states of the molecules, and in particular the solid-liquid interface, without any further assumptions. The price we have to pay is that the hydrodynamical quantities of interest, computed out of the microscopic state using the Irwing & Kirkwood (1950) prescriptions, need to be obtained under gravitational acceleration and thermal gradients much larger than those in real experiments.

On the Thermodynamics of Composition Graded Thermoelastic Solids

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We present a thermodynamic model describing the thermoelastic behavior of composition graded materials. The compatibility of the model with second law of thermodynamics is explored by applying a generalized Coleman-Noll procedure. The speeds of coupled first- and second-sound pulses, propagating either trough nonequilibrium or trough equilibrium states are derived. Several different types of perturbations, depending on the value of the material coefficients, are characterized. Under the assumption that the deformation of the body can produce changes in its stoichiometry, altering locally the material composition, the possibility of propagation of pure stoichiometric waves is pointed out. Thermoelastic perturbations generated by the coupling of stoichiometric and thermal effects are analyzed as well.

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Thermal Pulse Propagation beyond the Maxwell–Cattaneo theory: a Nonlinear Generalization

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According to the second law of thermodynamics, the entropy production has to be always non-negative in any point and at any time, whatever the thermodynamic process is [1], [2]. Since all solutions of the balance equations have to comply with the second law, that unilateral constraint is mainly used to determine the forms either of the constitutive relations [3], or of the evolution equations of the state-space variables.

In this talk we propose a non-local and non-linear thermodynamical model of heat transfer at nanoscale beyond the well-known Maxwell–Cattaneo theory. The compatibility of the proposed model with second law has been proved. The model is subsequently used to investigate the propagation of a heat pulse in one-dimensional nanosystems in the linear case. The predicted results are compared with those arising from the Maxwell–Cattaneo theory in order to point out the possible influence both of the non-local effects, and of the relaxation effects of the higher-order fluxes. Some problems related to initial data and boundary conditions are also discussed.

References

[1] S. R. De Groot, P. Mazur, *Non-equilibrium Thermodynamics*, North-Holland Publishing Company, Amsterdam, 1962.

[2] D. Jou, J. Casas-Vázquez, G. Lebon, *Extended Irreversible Thermodynamics*, 4th edn. Springer, Berlin, 2010.

[3] W. Muschik, H. Ehrentraut, *An amendment to the Second Law*, J. Non-Equilib. Thermodyn., 21, (1996), pp. 175–192.

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Linear and Nonlinear Models in Applied Mathematics

Effects of Temperature-Dependent Parameters on the Reflection of Thermoelastic Waves under Moore-Gibson-Thomson Heat Conduction

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This work discusses the reflection of thermoelastic waves under the Moore-Gibson-Thomson thermoelasticity theory [[1]], a generalized form of Green-Naghdi [[2]] and Lord-Shulman [[2]] theories. Owing to the realistic scenario, an isotropic medium with temperature-dependent elastic parameters is considered to study the plane waves. To highlight the nature of physical fields under the theory, analytical results along with a graphical representation for amplitude ratio and phase velocity for various waves are illustrated. Effects of empirical-index parameter and phase-lags are emphasized.

References

[1] Quintanilla R. Moore-Gibson-Thompson thermoelasticity. Math Mech Solids. 2019;24:4020-4031.

[2] Lord HW, Shulman Y. A generalized dynamical theory of thermoelasticity. J Mech Phys Solids. 1967;15:299-309.

[3] Green AE, Lindsay KA. Thermoelasticity. J Elast. 1972;2:1-7.

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Linear and Nonlinear Models in Applied Mathematics

Pinned Flexible Polymer under Oscillatory Linear Flow

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The non-equilibrium structural and dynamical properties of a flexible polymer pinned to a reflecting wall and subject to oscillatory linear flow are studied by numerical simulations. Polymer is confined in two dimensions and is modeled as a bead-spring chain while the interaction with the fluid is described by the Brownian multiparticle collision dynamics. At low strain the polymer is stretched along the flow direction. When increasing strain, chains are completely elongated and compressed against the wall when the flow is reverted. The conformations are analyzed and compared to the case of stiffer polymers [1]. The dynamics is investigated by looking at the motion of the center of mass which shows a frequency doubling along the shear direction.

References

[1] A. Lamura, R. G. Winkler, and G. Gompper, *Wall-Anchored Semiflexible Polymer under Large Amplitude Oscillatory Shear*, J. Chem. Phys. **154**, 224901 (2021).

Minisymposium
Linear and Nonlinear Models in Applied Mathematics

Fractal Mixtures for Heat Draining

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We present some recent results on the optimization of fractal interfaces to drain heat. Recent results and open problems will be discussed.

This is a joint project with M. Cefalo, S.Creo and Javier Rodriguez Cuadrado [1].

References

[1] M. Cefalo, S. Creo, M.R. Lancia, Javier Rodriguez Cuadrado, *Fractal mixtures for optimal heat draining*, To appear on Chaos and solitons, 2023.

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About the Zeros of the Lommel Functions

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The Lommel function $s_{\mu,\nu}$ are solutions of the following Bessel inhomogeneous diffferential equation

$$z^2\frac{d^2y(z)}{dz^2}+z\frac{dy(z)}{dz}+(z^2-\nu^2)y(z)=z^{\mu+1}$$

and play an important role in mathematical physics. In this talk, after recollecting some known properties of these functions, we give some recent results, including an integral representation and the distribution of the zeros of $s_{\mu,\nu}$ in the complex plane for certain values of the parameters μ and ν. Analytical and numerical aspects will be discussed.

MS3 - MATHEMATICAL AND NUMERICAL MODELLING OF POROUS MEDIA IN SUBSURFACE ENVIRONMENTS

Organizers: Marco Berardi, Fabio Di Fonzo, Matteo Icardi, Mario Putti

Modeling of subsurface processes has a significant impact in many applications in agricultural, environmental and engineering context. These processes will be treated both in a physically based way, and in a data-driven fashion, always in the framework of porous media. For instance, novel numerical methods will be considered, as well as machine learning techniques based on real-life data, and control approaches for managing irrigation will be faced in a theoretical framework and with a simulation point of view. Subsurface processes are characterized by high non-linearities and even discontinuities, sometimes memory terms in differential equations, mainly in advection-diffusion PDEs. This session will bring together applied mathematicians and hydrologists studying applied flow and transport processes, to discuss novel modelling and numerical approaches for facing these difficulties. In particular, contributions will span among new modeling approaches for describing root water uptake with memory terms, mass conservative numerical methods for transport equations, control techniques in unsaturated flow equations, data-driven approaches for salt transport in agricultural soils, heterogeneous reactions in porous media, etc.

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Minisymposium
Mathematical and Numerical Modelling of Porous Media in Subsurface Environments

A Preliminary Model for Optimal Control of Moisture Content in Unsaturated Soils

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We introduce an optimal control approach to Richards' equation in an irrigation framework, aimed at minimizing water consumption while maximizing root water uptake. We first describe the physics of the nonlinear model under consideration, and then develop the first-order necessary optimality conditions of the associated boundary control problem. We show that our model provides a promising framework to support optimized irrigation strategies, thus facing water scarcity in irrigation. The characterization of the optimal control in terms of a suitable relation with the adjoint state of the optimality conditions is then used to develop numerical simulations on different hydrological settings, that supports the analytical findings of the present study.

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FLOWS: A Physically-Based Model to Simulate Water Flow and Solute Transport in the Soil

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FLOWS (FLOw of Water and Solutes in soils) is a 1D physically-based model to describe water flow and solute transport in soil-plant-atmosphere systems. The numerical code, which was written in Matlab, simulates the vertical transient water flow by solving the 1D form of Richards Equation (RE). FLOWS also simulates solute transport by solving the 1D form of the Advection-Dispersion Equation (ADE). FLOWS solves RE using an implicit, backward, finite-difference scheme and solves ADE using an explicit central-difference scheme. FLOWS provides the temporal evolution along the soil profile of: soil water content, soil water pressure head, solute concentrations (including tracers, adsorbed, volatile and reactive solutes), water and solute uptake, actual transpiration by simulated crops (also accounting for water and osmotic stresses), soil-water fluxes, including deep percolation, and the related solute transport to runoff and drainage. FLOWS can be used to compute the optimal irrigation fluxes based on user-defined management parameters which are: the critical pressure head, hcrit, at which irrigation should start to bring the average pressure head, hav, to field capacity, as well as, the critical depth, zcrit, in which hcrit should be maintained. FLOWS can carry out multiple simulations which is useful for spatially distributed soil properties. The model also has a user-friendly Graphical User Interface (GUI) that allows user to manage large input files and view the main simulation outputs. FLOWS also simulates organic carbon, nitrogen and phosphorus (i.e., their transformations and transport) contextually to water contents and fluxes simulation.

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Understanding the Effects of Irrigation with Different Treatment Reused Waters: a Machine Learning Approach

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This talk presents some preliminary studies performed using selected data driven model to understanding the effects of irrigation with different treatment reused waters. Particularly, both exploratory data analysis and some data driven model generation will be presented to illustrate the studies conducted on a large dataset of soil data of an agricultural area which was collected by sensors at different depths and on soil parcels irrigated with different types of reused water. The aim of this analusis was to predict up to 72 hours of water content and soil salinity and understand how the involved variables behave in response to external factors such as irrigation and climate change. This understanding is important to regulate and plan usage of water resources.

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Mathematical and Numerical Modelling of Porous Media in Subsurface Environments

A Macroscopic Model for Unsaturated Flow in Deformable Evolving Porous Media

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In this work, we derive a model for a deformable porous medium with a growing interface and with phase change to model eco-hydro-mechanical problems in which there is a continuous deposition of porous substrate on the surface and the simultaneous decay and phase change between solid and fluid. The model will then be simplified for one-dimensional scenarios or in multi-dimension under small deformations, leading to a treatable set of equations. The time and length scales of the problem are discussed, and its limiting behaviour is discussed with the help of numerical simulations. Applications to environmental and manufacturing problems are discussed together with an overview of the split/partitioned numerical discretisation procedure for this coupled problem.

References

[1] AW Mahdiyasa, DJ Large, BP Muljadi, M Icardi, *Modelling the Influence of Mechanical-Ecohydrological Feedback on the Nonlinear Dynamics of Peatland*, Ecological Modelling, 2023. DOI: 10.1016/j.ecolmodel.2023.110299

[2] AW Mahdiyasa, DJ Large, BP Muljadi, M Icardi, S Triantafyllou, *MPeat – A fully coupled mechanical-ecohydrological model of peatland development*, Ecohydrology, e2361, 2021. DOI: 10.1002/eco.2361

[3] R Nuca, M Icardi, FA Radu, E Storvik, *Splitting Schemes for Coupled Systems of PDEs*, ArXiV preprint, 2023.

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Mathematical and Numerical Modelling of Porous Media in Subsurface Environments

Analytical and Numerical Solutions of Fractional Models in Porous Media

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In recent years, fractional partial differential equations (FPDEs) have played an important role in the modeling of physical and natural phenomena arising in many fields of the applied sciences. For example, these equations are increasingly used to model problems in fluid flow, diffusion and anomalous diffusion, reaction-diffusion, chemical physics, relaxation processes in complex systems, propagation of seismic waves, dynamical processes and porous structures and many other processes. It has been demonstrated that the fractional-order derivative represents an excellent instrument for the description of long memory and hereditary properties of various materials, systems and processes in comparison to integer-order derivation which lacks such effects. For this reason, the analytical and numerical solutions to these issues are seriously considered, and different analytical and numerical approaches and techniques have been developed to address them.

In this work, we present an approach to solving fractional diffusion–reaction equations in porous media defined in terms of the Riemann-Liouville and Caputo derivatives. The idea of solving these equations is based on the combination of the Lie symmetry theory, to reduce the given FPDE to a fractional ordinary differential equation (FODE), with the classical finite difference methods for solving the reduced equation. The proposed approach allows to determine solutions of FPDEs that may be difficult to find by their direct integration. The strong point of the approach is the low computational effort: solving a fractional ordinary differential equation leads to a lower cost respect to the integration of a FPDE. The numerical results demonstrate the efficiency, reliability and accuracy of the proposed procedure which turns out to be a good tool for solving a wide class of problems involving fractional differential equations.

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A Novel Reduced-order Model for Advection-dominated Problems Based on Radon-Cumulative-Distribution Transform

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Problems with dominant advection, discontinuities, travelling features, or shape variations are widespread in computational mechanics. However, classical linear model reduction and interpolation methods typically fail to reproduce even relatively small parameter variations, making the reduced models inefficient and inaccurate. In this work a novel reduced order modelling approach is proposed based on the Radon-Cumulative-Distribution transform (RCDT). We show that this non-linear transformation can significantly improve the dimensionality of proper orthogonal decomposition (POD) reconstructions and is capable of interpolating accurately some advection-dominated phenomena. The method is tested on various testcases in multiphase fluid dynamics.

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Numerical Simulation of a Compressible Gas Flow in Porous Media and Bioremendiation

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In a subsoil bioremediation intervention air or oxygen is injected in the polluted region and then a model for unsaturated porous media it is required, based on the theory of the dynamics of multiphase fluids in porous media.

In order to optmize the costs of the intervention it is useful to consider the gas as compressible and this fact introduces nonlinearity in the mathematical model.

The physical problem is described by a system of equations and the unknowns are: pollutant; bacteria concentration; oxygen saturation and oxygen pressure.

Then, by algebraic manipulations, the model is reduced a to a nonlinear system of partial differential equations describing: oxygen saturation, oxygen density and bacteria concentration.

For the proposed model, the results of some simulation experiments performed using COMSOL Multiphysics will be shown.

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Stabilized Explicit Methods for the Solution of a Vegetation Model

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In this talk, we focus on the numerical solution of a reaction-diffusion vegetation model that has been introduced in 2019 [2] to investigate the coexistence of two different plant species in arid environments (such as the African savannah), where there is scarce presence of water. This model is characterized by high stiffness, metastability, positivity and oscillating behavior in space. Our goal lies in the construction of efficient problem-oriented numerical schemes, which are able to preserve the a-priori known properties of the exact solution for large values of the discretization step-sizes.

For the numerical solution, we propose discretizations based on suitably modified non-standard finite differences (Mickens, 2020) combined with the TASE preconditioners (Calvo et al., 2021) and the exponential fitting technique (Ixaru, Vanden Berghe, 2004), proving that the methods thus derived are able to preserve the known properties of the model [1]. Finally, to increase the order of consistency of these schemes over time, we propose a generalization of the TASE-preconditioned methods by exploiting connections with the W-methods [3]. Numerical tests confirm the efficiency of the proposed techniques.

References

[1] D. Conte, G. Pagano, B. Paternoster., *Nonstandard finite differences numerical methods for a vegetation reaction-diffusion model.* J. Comput. Appl. Math., 2023.

[2] L. Eigentler, J. A. Sherratt, *Metastability as a coexistence mechanism in a model for dryland vegetation patterns.* Bull. Math. Biol., 2019.

[3] S. González-Pinto, D. Hernández-Abreu, G. Pagano, M.S. Pérez-Rodríguez, *Generalized TASE-RK methods for stiff problems.* Appl. Numer. Math., 2023.

MS4 - MMSEP: MODELLING, METHODS AND SIMULATIONS FOR ENVIRONMENTAL PROBLEMS

Organizers:

Carmela Marangi, Andrea Scagliarini, Luca Sgheri, Isabella Torcicollo

Climate change and landscape degradation in the Earth's Critical Zone are two of the most compelling issues our society must face daily. In recent years, the support of mathematics has firmly emerged as a valuable tool to understand, predict and possibly control such phenomena. The proposed Mini-Symposium aims at gathering scientists working at thedevelopment of mathematical models, computational methods and their applications to relevant environmental problems. Contributions are welcome from topics including (but not restricted to): Earth Observation based on data from remote sensors - Long Term Ecological Research on the structure and functions of ecosystems, oriented towards land degradation neutrality, Climate change impact on the Critical Zone, Biodiversity. - Diffusion of bacterial infections within plant species. Diffusion of invasive species within protected areas and agricultural areas. - Diagnostic and prognostic study of the Cryosphere (from alpine glaciers to polar sea-ice) - Pollutants Emission in urban freight transport versus delivery operational choices.

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Minisymposium
MMSEP: Modelling, Methods and Simulations for Environmental Problems

Pattern Formation Driven by Cross-diffusion in the Klausmeier-Gray-Scott Model

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Vegetation patterns are a characteristic feature of semi-deserts occurring on all continents. The Klausmeier-Gray-Scott 2D model for semi-arid ecosystems on a sloped terrain is considered with the addition of cross-diffusion terms. Pattern formation driven by cross-diffusion is studied in the resulting system.

References

[1] Christopher A. Klausmeier, Regular and Irregular Patterns in Semiarid Vegetation, Science 284, 1826–1828 (1999)

[2] Sjors van der Stelt, Arjen Doelman, Geertje Hek, Jens D.M. Rademacher, Rise and Fall of Periodic Patterns for a Generalized Klausmeier–Gray–Scott Model, J Nonlinear Sci (2013) 23:39–95

[3] Giancarlo Consolo, Gabriele Grifó, Giovanna Valenti, Dryland vegetation pattern dynamics driven by inertial effects and secondary seed dispersal, Ecological Modelling 474 (2022) 110171

[4] G. Gambino, M.C. Lombardo, M. Sammartino, Pattern formation driven by cross-diffusion in a 2D domain, Nonlinear Analysis: Real World Applications 14 (2013) 1755–1779

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MMSEP: Modelling, Methods and Simulations for Environmental Problems

Numerical Rock-Glacier Flow via the Pressure Method

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Recent literature confirms the crucial influence of non-viscous deformations together with temperature impact on glacier and rock glacier flow numerical simulation. Along this line, supported by the successful test on a one-dimensional set-up developed by two of the authors [2], we propose the numerical solution of a two-dimensional rock-glacier flow model based on an ice constitutive law of second grade differential type [1]. The procedure adopted uses a 2nd order finite difference scheme and imposes the incompressibility constrain up to computer precision via the pressure method, extended from newtonian computational fluid dynamics. The governing equations are solved in primitive variables with the advantage to avoid pre-/post-processing; splitted solution of the derived Poisson equation for pressure, source of undesired numerical mass unbalancing, is avoided as well. Numerical results will be shown.
The financial support of Piano Nazionale Ricerca Antartide (project PNRA16-0012) is acknowledged.

References

[1] Kannan, K., Mansutti, D., Rajagopal, K.R. and Urbini, S.: Mathematical modeling of rock glacier flow with temperature effects, in Mathematical Approach to Climate Change and its Impacts (P. Cannarsa, D. Mansutti and A. Provenzale, eds.), pp. 137-148, Springer-INDAM series, **38** (2020)

[2] Kannan, K., Mansutti, D. and Rajagopal, K.R.: Computational corroboration of the flow of rock glaciers against borehole measurements.Int. J. Non-lin. Mech., **132**, 103710 (2021)

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Investigating Spatial Patterns in a Model Describing Three-species Interactions

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A reaction-diffusion model with three interacting species, comprising a predator and a prey population that share the same resource [1, 2], is investigated. Differently from predation as traditionally defined, in this model a predator and its prey compete for a common resource (intraguild predation). To model the predator-prey interaction, and to better express the shape of the consumption rate, a Holling type II functional response is assumed. The equilibria of this model are found and their linear stability analytically studied. The species dispersion in the environment is investigated both analytically and numerically and the emerging of spatial patterns [3] discussed. This model can find practical applications in the context of biological control of invasive species.

References

[1] Safuan H.M., Sindhu H.S., Jovanoski Z., Towers I.N. (2013). Impact of biotic resource enrichment on a predator-prey population. *Bulletin of Mathematical Biology* 75 (10): 1798–1812. https://doi.org/10.1007/s11538-013-9869-7

[2] Capone, F., Carfora, M.F., De Luca, R., Torcicollo, I. (2018). On the dynamics of an intraguild predator–prey model. *Mathematics and Computers in Simulation* 149: 17–31. https://doi.org/10.1016/j.matcom.2019.03.010

[3] Carfora, M.F., Torcicollo, I. (2020). Cross-diffusion-driven instability in a predator-prey system with fear and group defense. *Mathematics* 8(8): 1244. https://doi.org/10.3390/MATH8081244

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Retrieval of Surface and Atmospheric Parameters from High Resolution Infrared Sensors

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Retrieval of surface and atmospheric temperature profiles together with gases concentrations is a fundamental problem in numerical weather prediction and Earth monitoring. In the last 20 years, the development of high-resolution infrared sensors able to be launched on satellites opened new opportunities for retrieval due to the unprecedented source of information they provide. The European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT), the National Oceanic and Atmospheric Administration (NOAA), the National Aeronautics and Space Administration (NASA), and other operational agencies are continuously developing product processing facilities to obtain L2 atmospheric profile products from infrared hyperspectral radiance instruments, such as the Infrared Advanced Sounding Interferometer (IASI), the Atmospheric Infrared Sounder (AIRS) or the upcoming Meteosat Third Generation – InfraRed Sounding (MTG-IRS). Nevertheless, infrared sensors cannot penetrate thick cloud layers, so observations are blinded to surface emissions under cloudiness; we can retrieve parameters only in clear-sky conditions. Therefore, the derived spatial fields will be flagged with missing data giving no continuity to inferred information and preventing the accurate modeling of energy fluxes between the surface and the atmosphere. From a mathematical point of view, the challenge is immense and expects a double step:

1) the retrieval of the L2 atmospheric profiles from L1 infrared radiances requires the inversion of the radiative transfer equation;

2)the reconstruction of a regular gridded L3 field from the L2 products demands interpolation techniques and spatial statistics to deal with large data sets.

This paper reviews and presents the physical modeling of radiative transfer in the atmosphere and the related mathematics of inversion in a form suitable for high spectral-resolution infrared sensors.

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The RothC Model: a Simple Tool for Simulating Soil Organic Carbon Dynamics

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In spite of its simple formulation (or perhaps because of it) the Rothamsted Carbon model (RothC) [1] is a versatile tool that allows to trace the evolution of the content of organic carbon in the subsoil. As it requires few environmental data, it is widely used both as stand-alone tool and as a component of more general land surface models. Initially introduced as a discrete monthly time-step procedure, it can be formulated in different ways, ranging from non-standard positive discrete map to fractional continuous differential system. With this simple model we will evaluate the effects of temperature, humidity and land cover variation on decomposition and storage of soil organic carbon for some real scenarios [2].

Acknowledgements. Funder: Project funded under the National Recovery and Resilience Plan (NRRP), Mission 4 Component 2 Investment 1.4 - Call for tender No. 3138 of 16 December 2021, rectified by Decree n.3175 of 18 December 2021 of Italian Ministry of University and Research funded by the European Union – NextGenerationEU; Award Number: Project code CN_00000033, Concession Decree No. 1034 of 17 June 2022 adopted by the Italian Ministry of University and Research, CUP B83C22002930006, Project title "National Biodiversity Future Center - NBFC".
Funder: European Union's Horizon 2.5-Climate-Energy and Mobility Programme, Restore 4Cs project under G.A. N.10156782.

References

[1] K. Coleman, D.S. Jenkinson *RothC-26.3 - A Model for the turnover of carbon in soil*, Evaluation of Soil Organic Matter Models, Springer Berlin Heidelberg 237–246, 1996.

[2] F. Diele, I. Luiso, C. Marangi, A. Martiradonna, E. Woźniak, *Evaluating the impact of increasing temperatures on changes in Soil Organic Carbon stocks: sensitivity analysis and non-standard discrete approximation.* Computational Geosciences, 26(5), 1345-1366, 2022.

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MMSEP: Modelling, Methods and Simulations for Environmental Problems

2D Model for Seismic Wave Propagation in Complex Fractured Domains

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Every year more than 50 high-intensity earthquakes, i.e. capable of producing damage to people or property, are recorded worldwide. Earthquakes cannot be predicted, so an accurate seismic risk assessment is mandatory. Numerical simulations obtained on reconstructed domains can certainly help, where analytical techniques do not provide satisfactory results or are simply not applicable. The analysis of seismic wave propagation in most cases requires the use of efficient numerical methods, especially in those subdomains of complex shapes, such as flood basins and faults, that are also inhomogeneous and/or contain fractures.
We investigate the seismic wave propagation in compex fractured domains. From the mathematical point of view the considered problem is described by linear wave equation with absorbing boundary conditions and non-welded contact conditions to model the fractures. For the numerical solution, we use similar techniques as in [1] together with Discontinuous Galerkin Spectral Element Method (DGSEM) as in [2].

References

[1] F. Di Michele, A. Styahar, D. Pera, J. May, R. Aloisio, B. Rubino, and P. Marcati *Fault shape effect on SH waves using finite element method*, Journal of Seismology, 26, 2022. - pp. 417-437.

[2] J. D. De Basabe, M. K. Sen, and M. F. Wheeler *Elastic wave propagation in fractured media using the discontinuous Galerkin method*, Geophysics, Vol. 81, No. 4, 2016. - pp. T163-T174.

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Minisymposium
MMSEP: Modelling, Methods and Simulations for Environmental Problems

Multiscale Modelling of Soil Bioremediation by Multispecies Biofilm

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A multiscale model for biofilm growth in a homogeneous porous medium is derived by upscaling the one-dimensional Wanner-Gujer multispecies biofilm model. The flow through the porous medium is assumed in a laminar and convection-dominated regime. The formal multiscale asymptotic method is applied to the mesoscale coupled system of elliptic-hyperbolic equations, which is a practical tool for determining the effective extent of various biofilm processes at the field scale. The proposed biofilm model is composed mainly of a dual-species biofilm subject to growth and loss due to substrate uptake and biomass detachment, respectively. The constructed model is a basic skeleton and the upscaling method is flexible to consider any number of bacteria species and substrates, and can be extended to various biofilm processes and kinetics (e.g., multiple substrates consumption, metals sorption and precipitation). The upscaling procedures end up with a stiff system of hyperbolic equations that are solved numerically. An original numerical code has been implemented on the MATLAB platform, based on the Uniformly accurate central scheme of order 2 (UCS2). To prove model consistency and highlight the main novelty of the work as compared to existing models, different simulation scenarios have been investigated by varying the following parameters: attachment velocity, detachment coefficient, and fluid flow rate. The mixed-culture biofilm assumption was found to significantly affect the overall system performance, and the model outputs qualitatively agree with the physical expectations.

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From Micro to Macro in the Physics and Ecology of Sea Ice

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Precipitously declining sea ice is impacting Earth's polar marine environments and their ecosystems, with ripple effects felt globally. As a material, sea ice exhibits complex composite structure over a broad range of length scales. A main challenge in modeling sea ice is how to use information on smaller scales to find effective behavior on larger scales relevant for climate and ecosystem models. Recovering small-scale parameters from bulk measurements is also of interest, as in remote sensing.
We will give an overview of recent advances on modeling sea ice [1], and organisms living in and on the ice. We consider the fractal geometry of the brine microstructure, percolation theory for fluid flowing through it, and the dynamics of algal communities living in the inclusions, using methods of uncertainty quantification [2]. Homogenization provides bounds on transport coefficients for EM waves in sea ice, ocean waves in the ice pack, and advection diffusion processes. We will discuss surface melt ponds and their fractal geometry, and energy minimizing pathways of polar bears traversing this environment. We consider PDE models and deep learning for the ice concentration field, and the fractal geometry of the marginal ice zone, the transitional region between the dense inner core of the ice pack and its outer fringes. This work is advancing how sea ice is represented in climate models, and improving projections of the future trajectory of Earth's sea ice packs and the ecosystems they support.

References

[1] K. M. Golden, et al., Modeling sea ice (invited), *Notices of the American Mathematical Society* 67(10), pp. 1535-1555 and issue cover, 2020.

[2] J. R. Reimer, et al., Uncertainty quantification for ecological models with random parameters. *Ecology Letters*, 25(10):2232–2244, 2022.

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Modelling Horizontal Gene Transfer of Plasmid-borne Resistance in Biofilms

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The global spread of antibiotic microbial resistance (AMR) is an increasing health concern, and has been mainly attributed to antibiotics abuse and misuse. Dissemination of AMR is largely associated to plasmids, extra-chromosomal genetic elements. Plasmid-carried resistance is transferred to new host cells through conjugation, which plays a crucial role in the ecological success of plasmids in bacterial communities. We present a mathematical model simulating the social behaviour of bacteria regulating plasmid transfer under selective pressure from metals or co-resistance and cross-resistance to antibiotics and metals. The model is formulated as a free boundary problem for a nonlocal system of PDEs with a convolution integral modelling the regulation of transfer genes expression. Gene expression is modelled as depending on the presence of potential receptors around a donor, called recipient-sensing. Dynamics of nutrients and metals is governed by reaction-diffusion PDEs. A promotion function is also introduced to account for the metal stimulation or inhibition on conjugation. Numerical simulations showed that the model is able to qualitatively reproduce the influence of conjugation on plasmid dynamics in a growing biofilm. In particular, the relative influence of conjugation and vertical gene transfer was compared, including the selective pressure exerted by the metals.

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On-off Intermittency in the Beddington-Free-Lawton Model

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In the recent literature the emergence of "on-off"intermittency has been observed in the Beddington-Free-Lawton host-parasitoid model, when system bifurcation parameters have stochastic (random) temporal variations [1]. Here we show the onset of "on-off "intermittency in a neighborhood of the free-parasitoid fixed point, for a random variation of the growth rate coefficient r. Moreover, we study the transmission of intermittency in coupled systems, by using the complex ecological networks formalism which provides a useful abstraction of ecological systems, representing them as graphs, composed of nodes (species) and edges (joint work with F. Diele, C. Marangi and A. Provenzale, [2]). In addition, we show what are the effects in terms of dynamics and emerging phenomenology when the environmental variability is modelled as a deterministic chaotic driving process (joint work with F. Diele and D. Lacitignola, [3]).

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References

[1] G. Vissio, A. Provenzale, *On-off intermittency and irruptions in host-parasitoid dynamics*, Journal of Theoretical Biology, 2022.

[2] A. Monti, F. Diele, C. Marangi, A. Provenzale, *The onset of intermittency in the Beddington-Free-Lawton model* (in preparation).

[3] D. Lacitignola, F. Diele, A. Monti, *On-off intermittency in a host-parasitoid model with a deterministic chaotic driver* (in preparation).

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Modelling Sea Ice and Melt Ponds Evolution: Sensitivity to Microscale Heat Transfer Mechanisms

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We present a mathematical model describing the evolution of sea ice and meltwater during summer. The system is described by two coupled partial differential equations for the ice thickness $h(x,t)$ and pond depth $w(x,t)$ fields. The model is similar, in principle, to the one put forward in [1], but it features i) a modified melting term, ii) a non-uniform seepage rate of meltwater through the porous ice medium and a minimal coupling with the atmosphere via a surface wind shear term, τ_s [2]. We test, in particular, the sensitivity of the model to variations of parameters controlling fluid-dynamic processes at the pond level, namely the variation of turbulent heat flux with pond depth and the lateral melting of ice enclosing a pond. We observe that different heat flux scalings determine different rates of total surface ablations, while the system is relatively robust in terms of probability distributions of pond surface areas. Finally, we study pond morphology in terms of fractal dimensions, showing that the role of lateral melting is minor, whereas there is evidence of an impact from the initial sea ice topography.

References

[1] M. Lüthje, D.L. Feltham, P.D. Taylor and M.G. Worster, *J. Geophys. Res.* **111**, C02001 (2006).

[2] A. Scagliarini, E. Calzavarini, D. Mansutti and F. Toschi, *Mathematical Approach to Climate Change and its Impacts. Springer INdAM Series* **38**, 179-198 (2020).

Minisymposium
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FORUM Sensitivity to Surface Emissivity

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FORUM (Far-infrared Outgoing Radiation Understanding and Monitoring) is a satellite mission selected in 2019 as the ninth ESA (European Space Agency) Earth Explorer mission. FORUM will provide interferometric measurements in the spectral interval encompassing the Far-InfraRed (FIR) part of the spectrum, responsible for about 50% of the outgoing longwave flux lost by our planet into space. While more accurate measurements of the Top Of the Atmosphere (TOA) resolved spectrum in the FIR are necessary for reducing uncertainty in climate models, existing instruments are insufficient. The observations will also improve the knowledge of several atmospheric variables, such as water vapor in the upper troposphere - lower stratosphere region, ice cloud properties and especially surface emissivity in the FIR, the focus of this seminar. In particular, I will present the results of our recent study of FORUM sensitivity in measuring surface emissivity in both clear and cloudy sky conditions, focusing on different aspects of the computational pipeline. Of particular interest are procedures for the injection of data from the ERA5 database, that is the fifth generation ECMWF (European Centre for Medium-Range Weather Forecasts) reanalysis for the global climate and weather, and Bayesian techniques for deriving a-priori estimates from the MODIS (Moderate Resolution Imaging Spectroradiometer) database. Finally, I will conclude by discussing extensions of the current surface emissivity database to IASI-NG (Infrared Atmospheric Sounding Interferometer New Generation) frequency range.

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Building a Realistic Simulation of the Atmospheric State in Radiative Transfer

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The usual way of conducting numerical experiments in a scientific problem consists in simulating and retrieving data using the same code. Unfortunately, often the operative conditions of the experiment cannot be simulated this way.

We show the details in the case of the inverse radiative transfer problem, which consists in retrieving an atmospheric state using experimental measurements of radiation intensities (spectra) from sounders.

The FORUM (Far-infrared Outgoing Radiation Understanding and Monitoring) instrument is a Fourier transform spectrometer that will fly as the ninth ESA's Earth Explorer mission, with expected launching date in 2027. The instrument will sound the far-infrared (FIR) and middle-infrared (MIR) part of the spectrum. The FIR region is responsible for about 50% of the outgoing longwave flux lost by our planet into space, but at the moment there is no instrument measuring the spectrally resolved radiance in this band.

To assess the capabilities of the instrument, a chain of codes has been set up and validated in the FORUM End-to-End simulator [1] ESA project. We present some results of this project and the last efforts to set up a realistic sandbox for testing retrieval algorithms and techniques before the actual flight of the instrument.

References

[1] L. Sgheri et al. *The FORUM end-to-end simulator project: architecture and results*, Atmospheric Measurement Techniques, 15, 573–604, 2022.

MS5 - MODELING, DESIGN OPTIMIZATION AND CONTROL IN SMART GRIDS

Organizers: Dhaker Abbes, Benoit Robyns

The main objective of the session is to inspect the mathematical methods/computational approaches to modeling, optimization and control of renewable energy sources to attain an optimized and a cost-effective solution in the context of smart grids. It emphasizes the theoretical background of research and development problems, both modeling and computational approches, covering all aspects which treat the following :

- Short term and long term load forecasting, electricity market forecasting, solar power forecasting, wind power forecasting (NN, NFIS, etc.)
- Multi-source systems optimization design (GA, SQP, Particle Swarm, Stochastic Optimization, etc.)
- Intelligent Energy management (EMS) (Fuzzy logic, Expert Systems, Game theory, etc.)
- Storage control and management (BMS),
- Operation of power system : unit commitment, hydro-thermal coordination, economic dispatch, congestion management, maintenance scheduling, state estimation, load and power flow, Remote monitoring, Power system automation, restoration, management, fault diagnosis, network security.

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Minisymposium
Modeling, Design Optimization and Control in Smart Grids

A Cooperative Distributed Droop Gains Adjustment in DC Microgrid

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Direct Current (DC) microgrids are a very promising solution to integrate renewable energy sources, energy storage systems and loads. The main goals of a microgrid controller are to achieve voltage regulation and load sharing among multiple distributed generation units (DGUs). Centralized controllers require high bandwidth communication while decentralised controllers suffer from poor performances. Distributed control techniques are more suitable to the distributed nature of microgrids [1].

Most of the existing distributed methods in the literature adjust the deviation caused by the conventional droop control by adding two additional terms. In this work, we propose a new cooperative distributed controller to adjust the droop gains of DGUs. The proposed method achieves average voltage regulation and proportional current sharing in a unified manner. It doesn't require additional corrective terms, resulting in a simple control structure. Moreover, it relies only on exchanging one communication variable among neighbor DGUs which reduces the communication burden. The stability of the proposed controller is analyzed using a small signal model of the system. The effectiveness of the proposed controller is evaluated under different operating conditions through Hardware-In-the-Loop (HIL) tests using NI PXIe real-time simulator.

References

[1] Espina, Enrique, et al. "Distributed control strategies for microgrids: An overview." IEEE Access 8 (2020): 193412-193448.

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Modeling, Design Optimization and Control in Smart Grids

Short-term Electricity Price Forecasting through Demand and Renewable Generation Prediction

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A fundamental characteristic of electricity prices in competitive markets is their extremely fluctuant behavior. This price volatility can have a large impact on the financial results of utilities and suppliers as it increases the risk of over or under contracting. The ability to forecast electricity prices from one to several days in advance can reduce this risk and help optimize the contracts for electricity trading companies in the day-ahead market or in derivative markets. Electricity price depends on many factors such as electricity demand, weather conditions (temperature, wind, rain), coal and gas prices, emissions costs, availability of generation units, etc. An ANN model for the forecasting of the hourly Market Clearing Price for the Spanish market from one to ten days in advance is presented in this paper. It can be considered a hybrid model composed of four different forecasting tools, three of them are based on the use of ANNs (wind, solar and price) while the demand forecasting model uses a similar-day approach with temperature correction. The results show that with a forecasting horizon of two days, the demand forecast has a 2.57 % rMAE, whereas the wind power forecast has a 12.96 % rMAE.. The price forecasts have a rMAE of 8.18 % when using a future market reference (MEFF) as an input and an 8.88 % when that input is removed. The model allows a market agent to correctly choose whether to participate in the daily market or in the futures markets a 69.9 % of the days..

References

[1] Jesus Lago, Grzegorz Marcjasz, Bart De Schutter, Rafał Weron, *Forecasting day-ahead electricity prices: A review of state-of-the-art algorithms, best practices and an open-access benchmark*, Applied Energy, Volume 293, 2021, ISSN 0306-2619.

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Modeling, Design Optimization and Control in Smart Grids

Coalitional Game-Based Gain Generation and Distribution for Collective Self-Consumption in an Energy Community

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Climate change is requiring changes in energy use. The integration of renewable energy sources into the energy mix is a viable solution for electricity generation, but their intermittence forces us to imagine new ways to consum and to distribute electricity. Thus, new economic models and new organizations have to be established. Energy communities are a recent legal solution to share renewable energy among local actors. Joining a community can allow participants to reduce their energy bill and environmental footprint. However the distribution of gains generated through collective self consumption is one of the main obstacles. An interesting possibility comes from the game theory, especially from cooperative game, as solutions concepts already exist to solve this kind of problem.

In this paper, a payoff distribution is proposed through a collaborative game. Two parrallel optimizations are established in order to compare the benefits of collective self consumption to individual self consumption. It is shown that the coordination of flexible devices to maximize the collective self-consumption rate generates gains on the electricity bill and environmental footprint. The aim of the study is then to explore ways to distribute these gains. Two major concepts in cooperative game theory are studied in this paper, the Shapley Value and the Nucleolus. The advantages and drawbacks of these concepts in an energy community context will be established. A methodology is proposed to permit a fairer distribution of payoffs according to specific energy management parameters such as efficiency and flexibility.

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Exploration and Optimisation of VoltagesPatterns Provided by a Multi-Active-Bridge with n Ports

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This paper presents a complete description of the switching sequences, as well as a piecewise modeling and optimization of the conduction and switching losses of an n-port Multi-Active-Bridge (MAB). The description presented analyzes all the voltage sequences (WVP aka Windings Voltages Patterns) generated by the multi-port version of the Triple Phase Shift strategy (which is the most general PWM technique for the well-known Dual Active Bridge [1]). This modulation allows us to control all the inter-legs/bridges phase shifts of the n ports. Within this framework, all switching sequences can be counted and systematically built. In this paper, the presented model is based on the WVP description and the aim of this study is to derive for all patterns the expressions of:

- power flows through all ports,
- currents in the transformer windings/switches (esp. peak and RMS values)

This modeling will then be used to explore optimal control values to reduce losses for a given power flow (specified power values at each port). Simulation results will be presented, as well as a comparison of the RMS currents generated and the number of Zero Voltage Switchings (ZVS) with Simple Phase Shift for a three-port converter

References

[1] HEBALA, O.M. 2020. Design and analysis of current stress minimalisation controllers in multi-active bridge DC-DC converters. Robert Gordon Uni- versity [online], PhD thesis. Available from: https://openair.rgu.ac.uk

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Modeling, Optimization and Management Strategies for a Microgrid with Integrated Thermal Energy Storage

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In order to reduce pollutants and greenhouse gases produced by conventional fossil fuels, and reduce energy expenditures making economic saving, a smart management of complex energy systems including energy sources, storage and loads is required. This work describes the mathematical model, the optimization, and an advanced management strategy of an electric microgrid connecting: a photovoltaic (PV) energy source; the electric grid; an electrochemical storage unit; and a Thermal Energy Storage (TES) system produced by Magaldi (Magaldi Green TES, MGTES) [1]. The MGTES system faces high heat load demands, typically supplied in traditional applications by fossil fuel fired generators, in the form of super-heat ed steam. Electric and thermal loads are connected to the microgrid. A model-based optimization is performed to define the optimal size of the microgrid components, and, in particular, the size of the PV system and the storage units. Then, the microgrid operating modes are analyzed and discussed, considering, in particular, the smart ones enabled by the storage systems. Finally, a smart management strategy minimizing the energy expenses is proposed, taking into account costs and production forecasts based on publicly available data. The management strategy is applied to the case study of a small industrial plant. [2].

References

[1] R. Acri, F. Bassetti, M. C. Falvo, L. Magaldi, M. Manganelli, L. Romagnoli, F. Santi, A. Scafuri, "A new thermal energy storage technology for power system services," *Proc. of IEEE ICPSE 2021*, doi = 10.1109/EEEIC/ICPSEurope51590.2021.9584535.

[2] P. Sharma, H.D. Mathur, P. Mishra, R.C. Bansal, "A critical and comparative review of energy management strategies for microgrids," *Applied Energy* 327(12), 120028, 2022.

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Modeling, Design Optimization and Control in Smart Grids

Artificial Intelligence and Blockchain for Decentralized Energy Management in an Energy Community of Smart Buildings

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The smart grid architecture has undergone significant changes with the introduction of renewable energy sources. Local energy communities (LECs) are emerging as a new solution to integrate these renewables into distribution networks by promoting peer-to-peer (P2P) energy exchanges between prosumers.
Prosumers, both energy producers and consumers, take part in LECs to optimize self-consumption, reduce energy costs, and minimize grid congestion. This project proposes a smart P2P market design for LECs, using artificial intelligence (AI) and blockchain technologies to promote self-consumption of locally produced energy and stimulate supply and demand balance within the community.
Building upon Matthieu STEPHANT's thesis on optimizing self-consumption in renewable energy communities using blockchain-based game theory [1], this project investigates a distributive method to optimize energy exchanges using AI based techniques such as deep learning and multi-agent systems. Our approach will explore the innovative combination of AI and blockchain based market design, compared to conventional centralized and decentralized management methods. Through analysis and simulation, we will assess the environmental impact of these solutions while highlighting the ability of AI to reduce this impact. Additionally, the project will investigate the relationship between AI and blockchain, assess energy costs, and improve the accuracy of electricity consumption and production forecasts.

References

[1] Stephant. M (2021). *Optimisation de l'autoconsommation dans une communauté énergétique locale via une blockchain (Doctoral dissertation, Paris, HESAM).*

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Optimizing Electric Bus Charging: Dynamic Tariffs in a Bi-level Framework Considering Weather Conditions and Energy Storage

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The steady growth of electric mobility, driven by the imperative to decarbonize the transportation sector, is particularly pronounced in bus-transit systems. However, the transition to fully electric bus networks faces infrastructure, operations, and grid integration challenges. Upgrading infrastructure for charging facilities requires substantial investments, while high charging power demands and uncertain charging events can strain the grid. A smart charging approach considering grid-bus system interaction and operational requirements is crucial to address these issues. In our previous work [1], we introduced a bi-level optimization model that incorporates dynamic time-differentiated pricing schemes to develop a coordinated charging routine for electric bus systems. Building upon this research, we extend our investigation to explore the impact of weather conditions on fleet energy requirements and consider the potential of buses acting as mobile energy storage systems during idle times. To provide realistic insights, we present a case study focusing on three routes and buses in Sherbrooke, Canada, where extreme weather conditions can highlight optimization needs, particularly in cold weather scenarios.

References

[1] Jônatas Augusto Manzolli, João Pedro F. Trovão, and Carlos Henggeler Antunes, Electric bus smart charging under a bi-level optimisation model to set dynamic tariffs, ECON 2022 48th Annual Conference of the IEEE Industrial Electronics Society, pp.1-6 (2022)

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Aerodynamic Models for Wind Turbines that Contribute to Grid Frequency Control

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The power extracted by the rotor of a wind turbine depends on the pitch angle of the blades. At high wind speeds, a controller limits its value. However, wind turbines that provide grid support may need to adjust the pitch angle in order to modify the generated power in response to frequency deviations.

An adequate aerodynamic model is necessary for such scenarios. The power coefficient is typically adjusted using two different equations. The most commonly used approach employs an analytic function with 10 coefficients (1). Alternatively, a polynomial expression with 25 coefficients is also utilized (2).

$$C_p = c_0\lambda + c_1\left(\frac{c_2}{\lambda_i} - c_3\beta - c_4\beta^{c_5} - c_6\right)e^{\frac{-c_7}{\lambda_i}}, \quad \lambda_i = \frac{1}{\frac{1}{\lambda+c_8\beta} - \frac{c_9}{\beta^3+1}} \tag{9}$$

$$C_p = \sum_{i=0}^{4}\sum_{j=0}^{4}\alpha_{i,j}\beta^i\lambda^j \tag{10}$$

The first model inaccurately represents the sensitivity of captured power to pitch variations found in real wind turbines, especially at high wind speeds and blade angles. It maintains a reduced sensitivity across the entire range of angles, which makes the inclusion of gain scheduling in captured power control unjustified, despite its presence in real wind turbines. This work proposes the use of the second model, as it allows for a more realistic control of captured power, which is beneficial when wind turbines contribute to frequency control.

On the other hand, all power coefficient models are static, meaning that a change in pitch angle leads to an instantaneous change in its value due to direct calculation. However, real wind turbines have shown that sudden variations in the pitch angle cause over-oscillations in the captured power. To address this, a dynamic model of a wind turbine has been developed in this work. Despite having limited aerodynamic information, this model ensures that varying the pitch angle causes the captured power to behave similarly to the measurements obtained from real wind turbines, which exhibit significant over-oscillations.

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Minisymposium
Modeling, Design Optimization and Control in Smart Grids

Multi-Agent Reinforcement Learning for Strategic Bidding in Two Stage Electricity Markets

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Our goal is to study the dynamics of electricity markets involving multiple competitive generators through multi-agent reinforcement learning (MARL) approaches. We start by formulating the electricity market as a two-stage stochastic game, involving a finite set of conventional and renewable energy producers, which bid on the day-ahead market, and an Independent System Operator (ISO), which is responsible for the clearing of the market. We assume that a predetermined part of the producers are non-strategic, bidding at their marginal costs, while the others might bid strategically trying to learn the outcome of the clearing. In the first stage, the strategic producers optimize simultaneously their bids by minimizing their expected costs (opposite of the expected profits), which is the difference between their production cost and the payment they receive from the ISO. The renewable energy producers' objective functions include a penalty assigning a cost to the imbalances caused by their forecast errors. In the second stage, the ISO receives the bids of all the producers. It clears the market by determining the activated volumes for each producer and a price minimizing the total cost under capacity constraints, including a conditional value at risk (CVaR) constraint for the renewable producers, capturing the risk aversion level that the requested volume violates their uncertain capacity. We derive closed form expressions for the producers' best-responses considering pay-as-clear and pay-as-bid as pricing schemes, and simulate the market dynamics, using MARL. To that purpose, we rely on modified versions of two actor-critic algorithms: Deep Deterministic Policy Gradient and Soft Actor-Critic. The simulations show how the producers adapt dynamically their strategies to learn the best bidding strategy, under limited information exchange. Finally, we identify conditions for the convergence of MARL algorithms to local equilibria of the stochastic game.

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Frequency Response of a 15 MW Offshore Wind Turbine for Low Frequency Stability Analysis

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Modelling of type-4 wind turbines for small signal stability analysis usually considers multiple simplifications, e.g. in many cases, the mechanical dynamics and the machine side converter are assumed as an ideal dc source that provides energy to the grid side converter. This paper proposes to include the overall wind turbine dynamics through a frequency analysis of a detailed wind turbine, including the complete wind turbine controller, as well as a non-linear wind turbine aeroelastic model, which includes the detailed dynamics of the tower, blades and mechanical drivetrain. Considering the mechanical model of the wind turbine allows the detecting of the low-frequency modes that can produce interactions with the wind turbine connected grid and that involve both electric, mechanical and aeroelastic modes. This detailed modelling approach is particularly important as there have been actual cases involving electromechanical coupling between the towers of different wind turbines transmitted though the electric grid. The computational load to carry out such frequency dependant models is relatively high, so the generator, the machine side converter, the grid side converter and the main grid are implemented in a real-time simulator so the identification in the low frequency range can be carried out in real-time frequency.

Finally, the results from the detailed model will be compared with the simplified ones, to quantify the level of accuracy of those simplifications, depending on the frequency range and operating point of each particular stability study.

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Pitch Control Design for Black-start Operation of a 15 MW Offshore Wind Turbine

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Black-start capability is particularly important for systems with a large scale renewable energy penetration. This capability is particularly relevant for the large amount of off-shore wind capacity planned to be installed in the North Sea.

Black-start capable wind turbines need to include grid-forming control on their grid side converters. This control would lead to operation below available power during the black-start process. However, pitch control for large wind turbines is usually designed for rated-speed rated-power operation.

As the wind turbine pitch-torque relation is non-linear, pitch controllers designed for rated-speed rated-power operation are suboptimal during the black-start process and might lead to excessive pitch actuation, overspeeding or even to wind turbine stall during large load increases.

This paper includes the design of a pitch controller for a large range of power and speed operational ranges typically found during black-start. The proposed controller will take into account an estimate of the operating point by means of power, speed and pitch angle measurements, thus not requiring knowledge of the wind speed for its operation.

Finally, a comparison between the new pitch controller and another one designed following the usual techniques shows the performance improvement of the new pitch controller during the black-start operation of a grid-forming wind turbine.

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Analysis of Non-uniform Grid-forming Control Techniques for the HVDC Connection of Renewable Energy

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Grid-forming control techniques are paramount for the high penetration of renewable energy generation. Existing research concentrates on the study of a specific grid-forming control strategy. However, realistic systems will include different grid-forming control strategies, which might be proprietary and, hence, not known.

Moreover, both the renewable energy generators and HVDC converters could have grid-forming capability.

Therefore, two important studies namely, stability and transient performance should consider the possibility of different grid forming control strategies on each system element (renewable energy converters and HVDC converters) and how these strategies would interact with each other.

Two different scenarios are considered, namely HVDC Diode Rectifier(DR) connected and VSC-HVDC connected wind power plants. For each scenario, both the wind turbine converters and the VSC-HVDC converters will consider a combination of different grid forming controllers (droop-based, advanced droop and Virtual Synchronous Machine based).

For all cases, it is shown that the parametrisation of the grid-forming controllers should consider other grid forming controllers to ensure good stability margins and adequate fault recovery.

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Multi-Objective Model for Residential Energy Management in Context of Renewable Communities

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The European Union strongly urged its member states to take action to establish energy communities. Domestic consumers now have the opportunity to organize themselves to play an active and decisive role in electricity supply chain and a solid contribution to an ecological footprint [1].

This work proposes the management of renewable resources in residential housing within the scope of participation in energy communities. A multi-objective optimization model will be developed to minimize electricity consumption and maximize self-consumption and participation (while as a prosumer) in an energy community. An energy storage system will be considered to optimize energy management. Actual data will be used to obtain realistic scenarios.

References

[1] P. N. Vasconcelos, G. S. Silva, A. C. Z. De Souza and B. I. Fuly, "Decentralized Governance and Energy Carbon Footprint: Opportunity for Re-Empowering People?," 2022 IEEE International Humanitarian Technology Conference (IHTC), Ottawa, ON, Canada, 2022, pp. 45-48, doi: 10.1109/IHTC56573.2022.9998383.

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Machine Learning Algorithms Applied to Smart Buildings with High Penetration of Electric Vehicles

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Our buildings demand a lot of energy and indirectly emit greenhouse gases. Cutting-edge technology can help reduce environmental impact. Smart building technology can save pollutants and expenses. In fact, they will be important in the future to tackle more than a third of the world's energy while combining Distributed Generation (DG) and the electric vehicle (EV) sector. In this context, accurately anticipating a smart building's car park usage will help to optimize energy use and benefit overall building management. Smart buildings aim to accurately anticipate the following day and hours in real-time.

This research uses machine learning methods to forecast smart building car park occupancy. This study examines machine learning systems to forecast EV park occupancy under different scenarios considering holidays periods. The model's pros and cons are examined. The proposed model is superior to the one proposed in [1] by Provoost et al., namely a accuracy higher than 80%.

References

[1] Provoost, J. C., Kamilaris, A., Wismans, L. J., Van Der Drift, S. J., Van Keulen, M. (2020). Predicting parking occupancy via machine learning in the web of things. Internet of Things, 12, 100301.

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Standby Thermal Management Methods and Hybrid Configuration for a Large Scale Vanadium Flow Battery

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Standby is a condition that may occur many times and for long periods in the operation of a Energy Storage System (ESS) based on Vanadium Flow Battery (VFB) for stationary energy storage services in smart grid, so that the efficient operation of these batteries calls for specific standby management procedures, with the aim to minimize losses while avoiding dangerous conditions. The first part of this work describes the characteristics of a standby thermal management system of a VFB capable of performing these tasks at a high efficiency for ESS based on a single VFB technology. Its design resorts to an experimental and numerical investigation that made use of a cell-resolved dynamic thermal model to determine the stack voltage, self-discharge and temperature evolution. Two different standby modes are analyzed: one with no continuous electrolyte flow (named "swamped standby mode") and the other with a small calibrated electrolyte cooling flow rate (named "streamed standby mode"). As regards the streamed standby mode, the optimal value of the cooling electrolyte flow rate minimizing self-discharge are identified and tested. Either one or the other can be adopted depending on the requested grid services. In the second part of this work, a further improvement in the reduction of self-discharge, while achieving a fast response time, is described by combining a supercapacitor energy storage technology with the VFB. Mathematical models of this hybrid storage system are conducted in Simulink environment, and a first analysis is presented [1].

References

[1] A. Trovò, M. Guarnieri "Standby thermal management system for a kW-class vanadium redox flow battery". Energ Conv Manag (2021), 226: 113510.

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Modeling, Design Optimization and Control in Smart Grids

Sizing of Storage under Uncertainty

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In order to implement energy storage with optimal operations and profits, the sizing of energy storage devices is essential. Storage devices must be sized and located considering power reliability, cost-effectiveness, and environmental-friendliness. Previous researchers have focused on handling RES uncertainty when dealing with the problem of storage sizing. The optimal ESS sizing problem is discussed in [1].
In this work, to identify the benefits of battery usage in terms of long-term benefits, and to take into account primary source (PV) generation in different seasons over one year, a storage sizing approach is proposed which applies the uncertainty analysis method. Historical databases of load demand and PV generation are analyzed with a probabilistic method to calculate the expected net demand during the day, taking into account the varying seasons and types of the day (workdays, non-workdays). This enables the building of PDF-based expected net demands that take into account the time factors (seasonal characteristics, national/regional holidays, etc.) of energy consumption and RESs generation. As a result, the sizing of storage is determined in order to save probable RES surplus.

References

[1] *S. Bahramirad, W. Reder, and A. Khodaei, "Reliability-Constrained Optimal Sizing of Energy Storage System in a Microgrid," IEEE TRANSACTIONS ON SMART GRID, vol. 3, no. 4, pp. 2056–2062, 2012.*

MS6 - MULTIVARIATE APPROXIMATION: NUMERICAL METHODS AND APPLICATIONS

Organizers: Costanza Conti, Stefano De Marchi, Elisa Francomano

Approximation is a well-studied mathematical topic, both from analytical and numerical points of view. Many problems of computational science, statistics, and probability require linear or nonlinear approximation, integration, or optimization of functions of many variables. Tensor networks, neural networks, and deep neural networks are the new tools for approximation especially in high-dimensional spaces. In a nutshell, the aim of approximation is to replace a target function, with a simpler one easy to evaluate and work with. Classical and modern approaches to this field cover various interesting techniques for multidimensional data and big data, information, signals, images, and so on.

The aim of this mini-symposium is to discuss both numerical aspects and the application of multivariate approximation since, in spite of its long tradition, many are open new problems like, for example, how to choose appropriate sampling sets for a given situation so that computations become tractable and the information loss is minimal or within acceptable tolerance limits.

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Minisymposium
Multivariate Approximation: Numerical Methods and Applications

Bivariate Spline Quasi-interpolants on Criss-cross Triangulations for the Approximation of Piecewise Smooth Functions

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Spline quasi-interpolation is well known to be a powerful and useful tool for the approximation of bivariate functions and data, important problem in many mathematical and scientific applications. If the function to be approximated is smooth, a spline quasi-interpolant is able to well reconstruct it, but if the function has jump discontinuities, the approximatingspline presents oscillations of magnitude proportional to the jump. Therefore, the aim of this talk is to apply Weighted Essentially Non-Oscillatory (WENO) techniques to modify classical quasi-interpolants in the space of C^1 quadratic and C^2 quartic splines on criss-cross triangulations, in order to avoid such oscillations. Using such a nonlinear modification we are able to avoid Gibbs phenomenon near discontinuities and, at the same time, maintain the high-order accuracy in smooth regions. We study the convergence properties of the proposed quasi-interpolants and we provide some numerical and graphical tests confirming the theoretical results.

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Multivariate Approximation: Numerical Methods and Applications

Nonlinear Quartic Quasi-interpolant Splines to Approximate Piecewise Smooth Functions

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Quasi-interpolation based on spline approximation methods is used in numerous applications. A quartic quasi-interpolating spline ([2]) is a piecewise polynomial of degree four satisfying C^3 continuity and five order of approximation, if the function to be approximated is sufficiently smooth. However, if the function has jump discontinuities, we observe that the Gibbs phenomenon appears when approximating near discontinuities. In this talk, we present nonlinear modifications of such a spline, based on weighted essentially non-oscillatory (WENO) techniques ([1]) to avoid this phenomena near discontinuities and, at the same time, maintain the five order accuracy in smooth regions. We also provide some numerical and graphical tests confirming the theoretical results.

References

[1] G-S Jiang and C-W Shu. Efficient implementation of weighted ENO schemes. *J. Comput. Phys.*, 126(1):202–228, 1996.

[2] P. Sablonnière. Univariate spline quasi-interpolants and applications to numerical analysis. *Rend. Sem. Mat. Univ. Pol. Torino*, 63:107–118, 2005.

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Minisymposium
Multivariate Approximation: Numerical Methods and Applications

MultiComponent Signals Interference Detection Exploiting HP-splines Frequency Parameter

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MultiComponent Signals (MCSs) play a key role in many different fields such as biology and medicine, in audio processing, in civil and military air traffic control and security, in seismology, in physics etc. [1]. This kind of signals has an effective representation (spectrogram) in the time-frequency plane and is mainly characterized by Instantaneous Frequency (IF) curves (ridges). Usually, ridges detection becomes very hard for interfering signals. That's why interference regions detection in the spectrogram becomes a crucial step for an effective IF analysis [2]. We present preliminary results concerning a data-driven approach in which the frequency parameter of an hyperbolic-polynomial penalized spline (HP-spline [3]), suitable designed for the signal regression, may help to detect the interference regions in the corresponding spectrogram. More specifically, the approximation error by the HP-spline of the spectrogram variations along scales results high in correspondence to interference regions because of a very low (and an analytically unpredictable) regularity in these regions, thus resulting in a possible indicator of the presence of interference. Some preliminary numerical experiments show that the proposed approach properly detects interference of different kinds of MCSs.

References

[1] S. Mallat, A wavelet tour of signal processing, Elsevier: Amsterdam, The Netherlands, 1999.

[2] V. Bruni, M. Tartaglione, D. Vitulano, *Skeleton-based reassignment of nonstationary signals spectrogram*, Digital Signal Processing, Volume 128, August 2022.

[3] R. Campagna, C. Conti, Penalized hyperbolic-polynomial splines, Applied Mathematics Letters, Volume 118, 2021.

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Minisymposium
Multivariate Approximation: Numerical Methods and Applications

Time-frequency Interpolation of Wavelet Scattering Coefficients for Signal Classification

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Wavelet scattering (WST) is a time-frequency transform that shares the convolutional architecture with convolutional neural networks, but it allows for a faster training and it often needs smaller training sets [1]. WST showed to be a powerful tool for signal classification whenever embedded in a machine learning architecture [2]. One of the most delicate parameters in convolutional architectures is the stride (temporal sampling) parameter that strongly affects the computational load as well as the classification rate. In this work the role of sampling in the wavelet scattering transform is studied for signal classification purposes. Subdivision schemes [3] are properly tuned to compensate the information lost when using sampling at each layer of the transform. Preliminary results show that interpolating subdivision schemes allow to define a set of features that improve the classification rates provided by the conventional WST.

References

[1] J. Anden, S. Mallat, *Deep Scattering Spectrum*, IEEE Transactions on Signal Processing 2014.

[2] V. Bruni, M.L. Cardinali, D. Vitulano, *An MDL-based Wavelet scattering features selection for signal classification*, Axioms, 2023.

[3] N. Dyn, D. Levjn, *A 4-point interpolatory subdivision scheme for curve design*, Computer Aided Geometric Design, 1987.

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Multivariate Approximation: Numerical Methods and Applications

Predictive Modeling of Soil Microbiota Growth Using PINN

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This study aims to predict the growth of microbial populations within the soil using tools like Physics Informed Neural Networks (PINN), overcoming challenges in molecular analysis of individual samples such as the Great Plate Count Anomaly and the general unculturability of soil bacteria. PINN can be used to model the growth of bacterial and fungal populations, considering environmental factors like temperature, solar radiation, air humidity, soil hydration status, and external weather conditions. By utilizing field data and applying equations that describe the biological mechanisms of microbial growth, a PINN was trained to predict the development of the microbiota over time. PINN can also be used to forecast the microbiota's evolution under different environmental conditions, such as global warming due to climate change or variations in nutrient availability. The results demonstrate that the use of PINN for studying microbial growth and evolution is a promising tool for enhancing agriculture, optimizing cultivation processes, and facilitating efficient resource management.

References

[1] Boswell, G.P., Jacobs, H., Ritz, K. et al. *The Development of Fungal Networks in Complex Environments.* Bull. Math. Biol. 69, 605–634 (2007). https://doi.org/10.1007/s11538-005-9056-6

[2] Du H, Tran TB, Perré P. *A 3-variable PDE model for predicting fungal growth derived from microscopic mechanisms.* J Theor Biol. 2019 Jun 7;470:90-100. doi: 10.1016/j.jtbi.2019.03.015. Epub 2019 Mar 21. PMID: 30905712.

[3] Euan T Smithers and others, *Mathematical principles and models of plant growth mechanics: from cell wall dynamics to tissue morphogenesis*, Journal of Experimental Botany, Volume 70, Issue 14, 1 July 2019, Pages 3587–3600, https://doi.org/10.1093/jxb/erz253

[4] Cuomo, S., Di Cola, V.S., Giampaolo, F. et al. *Scientific Machine Learning Through Physics–Informed Neural Networks: Where we are and What's Next.* J Sci Comput 92, 88 (2022). https://doi.org/10.1007/s10915-022-01939-z

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Multivariate Approximation: Numerical Methods and Applications

On the Numerical Solution of Some Elliptic PDEs with Neumann Boundary Conditions through Multinode Shepard Method

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In this talk, the multinode Shepard method is proposed to solve elliptic partial differential equations with Neumann boundary conditions. The method has been opportunely handled to solve different equations with various boundary conditions dealing with scattered distribution of points [1, 2]. The particular feature of the method, based on local polynomial interpolants on opportunely choosen nearby nodes [3], is a collocation matrix which is reduced in size with many zero entrances and a small condition number. Experiments in 2d domains have been performed with Neumann boundary conditions. Comparisons with the analytic solutions and the results generated with the RBF method proposed by Kansa are presented referring to different distribution of points.

References

[1] F. Dell'Accio, F. Di Tommaso, O. Nouisser, N. Siar, *Solving Poisson equation with Dirichlet conditions through multinode Shepard operators*, Comput. Math. with Appl., 98 (2021), 254–260.

[2] F. Dell'Accio, F. Di Tommaso, G. Ala, E. Francomano, *Electric Scalar Potential Estimations for Non-Invasive Brain Activity Detection Through Multinode Shepard Method*, MELECON 2022 - IEEE Mediterranean Electrotechnical Conference, Proceedings, (2022), 1264–1268.

[3] L. Bos, S. De Marchi, A. Sommariva, M. Vianello, *Computing multivariate Fekete and Leja points by numerical linear algebra*, SIAM J. Numer. Anal., 48 (2010), 1984–1999.

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Multivariate Approximation: Numerical Methods and Applications

Simple Strategies for Approximating Scattered Data and Functions

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Multivariate (scattered) data approximation problems come out in various applications and, in this sense, are one of the most attractive research topics in applied mathematics, numerical analysis, engineering, data science and in all those fields that need to treat (big) data. Many methods have already been proven to be effective numerical tools, such as multivariate splines, Radial Basis Functions (RBFs) and in some sense also finite elements. In this talk we confine ouselves to RBF approximation which is a popular tool for scattered data approximation and meshless methods. We present three simple approaches that turn out to work very well in those frameworks.

- the *rescaled* method for RBF approximation of functions [1];
- the *mapped bases without resampling* method, applied both for mitigating the Runge and Gibbs phenomena [2];
- the *variably scaled discontinuous kernels*, for functions having discontinuities and image reconstructiion [3];

References

[1] S. De Marchi, A. Idda and G. Santin, A rescaled method for RBF approximation, Proceedings of "Approximation Theory XV" (2017).

[2] S. De Marchi, F. Marchetti, E. Perrracchione and D. Poggiali:, Polynomial interpolation via mapped bases without resampling, J. Comput. Appl. Math. 364 (2020), p.112347

[3] S. De Marchi, F. Marchetti and M. Perracchione, Jumping with Variably Scaled Discontinuos Kernels (VSDK), BIT Numerical Mathematics 60 (2020), pp. 441-463.

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Multilevel and Progressive Iterative Methods for Approximation and Numerical Integration

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Recently two kinds of approximation techniques have been introduced and studied in the literature. As far as we know, both seminal papers [1, 2], one dealing with the so-called *multilevel approximation* (MA) and the other one with the so-called *progressive iterative approximation* (PIA), were published in 2004. They are two different ways of triggering an iterative procedure, acting on some kind of remainder (or error) in the base method.

Induced by these ideas, we are interested in investigating and comparing both techniques MA and PIA, when applied to spline QI operators on bounded domains, in particular to the well known variation-diminishing Schoenberg-Marsden operator, suitably modified in order to satisfy the main interest that lies in providing best approximation order, while being easy to compute.

This study is also aimed at defining new quadrature formulas, based on such iterative techniques.

References

[1] L. Ling, *A univariate quasi-multiquadric interpolation with better smoothness.* Computers and Mathematics with Applications 48 (2004), 897-912.

[2] H. Lin, G. Wang, C. Dong, *Constructing iterative non-uniform B-spline curve and surface to fit data points*, Science in China (Series F) 47 (2004), 315-331.

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Minisymposium
Multivariate Approximation: Numerical Methods and Applications

Deep Mapping Techniques for Solving Time-Fractional PDEs Containing Crack and/or Corner Singularities

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In the paper [1], the Non-Uniform Rational B-Spline geometrical mapping, referred to as NURBS singular mapping, was introduced as a technique to handle singularities arising from Partial Differential Equations (PDEs) on domains containing cracks and/or corners. This approach shares similarities with the Method of Auxiliary Mapping (MAM). The main idea of the NURBS singular mapping and MAM is to define a geometrical mapping that generates point singularity functions based on the parametrization of circular arcs and NURBS, respectively. We propose a new type of mapping technique called Deep Mapping Technique (DMT) based on a neural network. The DMT is a nonlinear function generated by deep learning and learns the behaviors of the NURBS singular mapping and MAM. We use the DMT combined with the Physics-Informed Neural Network (PINN) to deal with Time-Fractional PDEs (TF-PDEs) containing cracks and/or corners in the physical domain. The performance of the proposed method is measured by comparing it with the method introduced in the paper [2].

References

[1] J. W. Jeong, H.-S. Oh, S. Kang, H. Kim*Mapping techniques for isogeometric analysis of elliptic boundary value problems containing singularities*, Computer Methods in Applied Mechanics and Engineering, 254 (2013) 334–354

[2] B. Jang, H. Kim*Mapping techniques for collocation method of time-fractional convection-diffusion equations in domains with cracks*, submitted to the Mathematics and Computers in Simulation

Minisymposium
Multivariate Approximation: Numerical Methods and Applications

A Collocation Method for the Space-time Fractional Diffusion Problem

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Nowadays, fractional differential equations are often used to better model real phenomena in various fields of sciences (e.g. biology, physics, mechanics, economics, control theory, etc). We consider the discretization of the space-time fractional diffusion problem, where the fractional derivative in time is considered in the Caputo sense, and the fractional diffusion is represented by the Riesz-Caputo derivative. This is a natural choice due to the symmetry properties of the Riesz-Caputo operator [1]. A collocation method is introduced based on a B-spline representation of the solution, where the symmetry properties of both the spline basis functions and the Riesz–Caputo operator are exploited to provide an efficient method for solving the proposed fractional differential problem.

References

[1] F. Pitolli, C. Sorgentone, E. Pellegrino, *Approximation of the Riesz-Caputo derivative by cubic splines*, Algorithms 15 (69), 2022.

MS7- NUMERICAL METHODS FOR FRACTIONAL-DERIVATIVE DIFFERENTIAL EQUATIONS

Organizers: Roberto Garrappa, Martin Stynes

At present the numerical solution of problems involving fractional-order derivatives is a "hot" research area; a search of the MathSciNet database using MSC Primary = 65 (numerical analysis) and Anywhere = "fractional derivative" yields 791 papers for the period 2018-2023. Numerical analysts are interested in this topic because fractional derivatives are increasingly used in modelling applications and they are sufficiently different from classical integer-order derivatives so as to require new numerical methods; furthermore, the error analysis of these new methods can be challenging.

This minisymposium welcomes talks on numerical methods (finite differences, finite elements, spectral methods,...) for discretising fractional-derivative differential equations that pay some attention to rigorous error analysis. Because this research area is very active, it is important that presenters of talks are familiar with recent developments. The organizers invite abstracts that show an awareness of current activity in the area and present some new development in the topic of the minisymposium.

Minisymposium
Numerical Methods for Fractional-derivative Differential Equations

A Rational Preconditioner for Multi-dimensional Riesz Fractional Diffusion Equations

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In this talk we propose a rational preconditioner for an efficient numerical solution of linear systems arising from the discretization of multi-dimensional Riesz fractional diffusion equations. In particular, the discrete problem is obtained by employing finite difference or finite element methods to approximate the fractional derivatives of order α with $\alpha \in (1, 2]$. The proposed preconditioner is then defined as a rational approximation of the Riesz operator expressed as the integral of the standard heat diffusion semigroup. We show that, being the sum of k inverses of shifted Laplacian matrices, the resulting preconditioner belongs to the generalized locally Toeplitz class, a wide algebra of matrix sequences that can be linked to a function representing the asymptotic eigenvalue distribution as the matrix size diverges. As a consequence, we are able to provide the asymptotic description of the spectrum of the preconditioned matrices and we show that, despite the lack of clustering just as for the Laplacian, our preconditioner for α close to 1 and $k \neq 1$ reasonably small, provides better results than the Laplacian itself, while sharing the same computational complexity.

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Minisymposium
Numerical Methods for Fractional-derivative Differential Equations

Numerical Solution of Random Fractional Laguerre-type Differential Equations via Moments and Density

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In this work we construct convergent analytic-numerical approximations for the following class of random fractional Laguerre-type differential equations:

$$\begin{cases} (1-t^2)({}^C D_0^\alpha X)(t) - 2tX'(t) + LX(t) = 0, \quad 1 < \alpha < 2, \\ X(0) = C_0, \\ X'(0) = C_1. \end{cases} \tag{11}$$

Here, $({}^C D_0^\alpha X)(t)$ is the Caputo fractional derivative of order α of $X(t)$ and $X'(t)$ the classical first order derivative. The variables C_0, C_1 and L are assumed second order random variables defined in a complete probability space.

A main challenge appearing in our analysis is that the equation combines random fractional Caputo and classical derivatives.

We construct analytic-numerical approximations by representing the solution as a random double series $X(t) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} X_{m,n} t^{m+\alpha n}$. The coefficients $X_{m,n}$ are recursively obtained applying a generalized version of the random Frobenius method. Since no explicit expression can be derived from $X_{m,n}$, in this work, we develop a computational method to approximate the first, second and third statistical moments of the solution, which is a stochastic process. From this key information, we take advantage of the Principle of Maximum Entropy to construct reliable approximations of the probability density function of the solution.

Several numerical examples, where different probability distributions are chosen for the random parameters, are show.

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Minisymposium
Numerical Methods for Fractional-Derivative Differential Equations

Two Kinds of Numerical Algorithms for Ultra-slow Diffusion Equations

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In this article, two kinds of numerical algorithms are derived for the ultra-slow (or superslow) diffusion equation in one and two space dimensions, where the ultra-slow diffusion is characterized by the Caputo-Hadamard fractional derivative of order $\alpha \in (0,1)$. To describe the spatial interaction, the Riesz fractional derivative and the fractional Laplacian are used in one and two space dimensions, respectively. The Caputo-Hadamard derivative is discretized by two typical approximate formulae, i.e., L2-1_σ and L1-2 methods. The spatial fractional derivatives are discretized by the 2-nd order finite difference methods. When L2-1_σ discretization is used, the derived numerical scheme is unconditionally stable with error estimate $\mathcal{O}(\tau^2 + h^2)$ for all $\alpha \in (0,1)$, in which τ and h are temporal and spatial stepsizes, respectively. When L1-2 discretization is used, the derived numerical scheme is stable with error estimate $\mathcal{O}(\tau^{3-\alpha} + h^2)$ for $\alpha \in (0, 0.3738)$. The illustrative examples displayed are in line with the theoretical analysis [1].

References

[1] M. Cai, C.P. Li, Y. Wang, *Two kinds of numerical algorithms for ultra-slow diffusion equations*, submited.

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Minisymposium
Numerical Methods for Fractional-Derivative Differential Equation

A Computational Approach for Variable-order Fractional Differential Equations

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Recently, new integrals and derivatives of fractional and variable order have been obtained by generalizing usual operators in the Laplace transform domain rather than in the time-domain [1]. One of the main advantages of pursuing the generalization of constant-order operators in the Laplace transform domain is that they naturally satisfy a Sonine condition which is essential to obtain integrals and derivatives inverting one each other.

However, this approach leads to operators defined as convolution integrals with kernels without an explicit analytical formulation. Numerical methods are therefore mandatory to handle these operators and solve corresponding fractional differential equations of variable-order.

In this talk we discuss few theoretical aspects of variable-order fractional differential equations in this framework and we focus on the application of Convolution Quadrature Rules proposed by Lubich in [3]. Since quadrature weights are not analytically known, they must be computed by means of specific quadrature rules in the complex plane [2]. Moreover, to reduce error propagation, quadrature rules must be evaluated with high precision and therefore a detailed error analysis is introduced to select quadrature parameters.

References

[1] R. Garrappa, A. Giusti, F. Mainardi, *Variable-order fractional calculus: a change of perspective*, Commun. Nonlinear Sci. Numer. Simul., 2021, 102, 105904.

[2] R. Garrappa, A. Giusti, *A computational approach to exponential-type variable-order fractional differential equations*, Submitted, 2023.

[3] C. Lubich, *Convolution quadrature and discretized operational calculus I, II*, Numer. Math., 1988, 52, 129-145, 413-425.

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Minisymposium
Numerical Methods for Fractional-Derivative Differential Equations

Numerical Approximation of a Differential Equation with a Riemann-Liouville-Caputo Fractional Derivative

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An initial-boundary value problem is considered whose highest-order space derivative is a Riemann-Liouville-Caputo fractional derivative of order $\alpha \in (1, 2)$. This type of fractional derivative has been used, for example, in [1], [2], [3] and [4]. Some properties of the solution are discussed and, in particular, it is shown that it has a weak singularity in the left side of the domain, i.e., near $x = 0$. The solution is approximated using a finite difference scheme on a uniform mesh and the weakly singular behaviour of the solution is taken into account in the error analysis. It is proved that the scheme converges with almost first order (except for a logarithmic factor) in the maximum norm. Numerical results are given that corroborate our theoretical results.

References

[1] B. Baeumer, M. Kovács, M.M Meerschaert, and H. Sankaranarayanan, Boundary conditions for fractional diffusion. J. Comput. Appl. Math. 336 (2018), 408–424.

[2] J.L. Gracia, E. O'Riordan, and M. Stynes, Convergence analysis of a finite difference scheme for a two-point boundary value problem with a Riemann-Liouville-Caputo fractional derivative. BIT 60 (2020), no. 2, 411–439.

[3] J.L. Gracia, and M. Stynes, A finite difference method for an initial-boundary value problem with a Riemann-Liouville-Caputo spatial fractional derivative. J. Comput. Appl. Math. 381 (2021), Paper no. 113020, 14 pp.

[4] J.F. Kelly, H. Sankaranarayanan, and M.M. Meerschaert, Boundary conditions for two-sided fractional diffusion. J. Comput. Phys. 376 (2019), 1089–1107.

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Minisymposium
Numerical Methods for Fractional-Derivative Differential Equations

Nonuniform Time-stepping Approximation Methods to Solve the Two-dimensional Time-fractional Diffusion-wave Equation

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In this article, we discuss two numerical methods for solving the one and two-dimensional time-fractional diffusion-wave equation. The time-fractional derivative is chosen in the Caputo sense. We use the Nonuniform $L1$ method and Nonuniform $L1-2$ method, to approximate the time-fractional Caputo derivative (TFCD) of order α $(1 < \alpha < 2)$. To handle the weak singularity at $t = 0$, the TFCD is discretized on the nonuniform temporal mesh. Adopting these two approximation methods for TFCD and central difference operator for approximation of the space derivative to find the system of algebraic equations. After that, the system of equations is solved by using the Alternating Direction Approach. The numerical results shows that both schemes are efficiently accurate. The Nonuniform $L1$ scheme has $\min(3-\alpha, \gamma\alpha)$ temporal convergence order and second-order in space, where γ is the mesh grading parameter used in the construction of the nonuniform mesh. The Nonuniform $L1-2$ scheme has second-order accuracy in both time and space. We plotted the absolute error graphs to show the advantage of nonuniform meshes near singular point $t = 0$.

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Numerical Methods for Fractional-Derivative Differential Equations

Fast Second-order Numerical Method for Variable-order Caputo Fractional Differential Equations

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In this work, we propose a fast and second-order numerical method for solving the Caputo variable-order(VO) time fractional diffusion equation based on a $\mathcal{L}2\text{-}1_\sigma$ method [1] and "SBBP" algorithm [2]. For the Caputo VO function $\alpha(t)$, the sum of exponential (SOE) calculation of the kernel function that is an efficient algorithm to reduce computational complexity, requires approximating the points and weights at every time step. Here we employ the shifted binary block partition (SBBP) to decompose the integral in the derivative and approximate the scaled kernel function in each sub-intervals by polynomials of degree r whose computational complexity is $\mathcal{O}(rn \log n)$. But it has a low convergence order of $\mathcal{O}(\Delta t^{2-\bar{\alpha}})$, where $\bar{\alpha} = ||\alpha(t)||_\infty$. We propose a new $\mathcal{L}2\text{-}1_\sigma$ that has a convergence of $\mathcal{O}(\Delta t^{3-\bar{\alpha}})$ and apply it to approximate the Caputo variable-order(VO) time fractional diffusion equation. The stability and the error analysis has been proved. Several numerical results show the effectiveness of the proposed method and demonstrate the accuracy and performance of the theory.

References

[1] A. A. Alikhanov, A new difference scheme for the time fractional diffusion equation, Journal of Computational Physics, 280 (2015) pp. 424-438.

[2] Z. W. Fang, H. W. Sun and H. Wang, A fast method for variable-order Caputo fractional derivative with applications to time-fractional diffusion equations, Computers & Mathematics with Applications, 80 (2020), pp. 1443-1458.

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Minisymposium
Numerical Methods for Fractional-Derivative Differential Equations

An Efficient Computational Technique for 2D Time-Fractional Diffusion Problem

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In this article, the alternating direction implicit type operator splitting [1] discontinuous Galerkin finite element method [2, 3] is proposed to numerically solve a class of two-dimensional time-factional diffusion equation. The time-fractional derivative term is discretized over a non-uniform mesh using the well known $L2$-scheme and for the discretization of the spatial derivatives, the discontinuous Galerkin finite element method is used in both x and y directions over the uniform mesh. The stability and the error estimate of the proposed scheme are addressed. Finally, we give some numerical experiments to show the efficiency of the proposed method.

References

[1] A. Das, S. Natesan. A novel two-step streamline-diffusion FEM for singularly perturbed 2D parabolic PDEs. *Applied Numerical Mathematics*, 172: 259–278, 2022.

[2] B. Rivière, *Discontinuous Galerkin methods for solving elliptic and parabolic equations*, Frontiers in Applied Mathematics Vol. 35, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, 2008.

[3] G. Singh, S. Natesan Superconvergence of discontinuous Galerkin method with interior penalties for singularly perturbed two-point boundary-value problems. *Calcolo*, 55(54), 2018.

Minisymposium
Numerical Methods for Fractional-derivative Differential Equations

Optimal Long-time Decay Rate of Solutions of Complete Monotonicity-preserving Schemes for Nonlinear Time-fractional Evolutionary Equations

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The solution of the nonlinear initial-value problem $\mathcal{D}_t^\alpha y(t) = -\lambda y(t)^\gamma$ for $t > 0$ with $y(0) > 0$, where $\mathcal{D}_t^\alpha$ is the Caputo derivative of order $\alpha \in (0,1)$ and λ, γ are positive parameters, is known to exhibit $O(t^{-\alpha/\gamma})$ decay as $t \to \infty$. No corresponding result for any discretisation of this problem has previously been proved. We shall show that for the class of complete monotonicity-preserving schemes (which includes the L1 and Grünwald-Letnikov schemes) on uniform meshes $\{t_n := nh\}_{n=0}^\infty$, the discrete solution also has $O(t_n^{-\alpha/\gamma})$ decay as $t_n \to \infty$. For the L1 scheme, the $O(t_n^{-\alpha/\gamma})$ decay result is shown to remain valid on a very general class of nonuniform meshes. Our analysis uses a discrete comparison principle with discrete subsolutions and supersolutions that are carefully constructed to give tight bounds on the discrete solution. Numerical experiments confirm our theoretical analysis.

Full details are given in [1].

References

[1] D. Wang & M. Stynes, Optimal long-time decay rate of solutions of complete monotonicity-preserving schemes for nonlinear time-fractional evolutionary equations, SIAM J. Numer. Anal. (to appear).

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Minisymposium
Numerical Methods for Fractional-derivative Differential Equations

A Stabilizer-free Weak Galerkin Finite Element Method for the Distributed Order Time-fractional Diffusion Equation

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We consider the following distributed order time-fractional diffusion equation with the Dirichlet boundary conditions

$$\begin{aligned}
&\mathcal{D}_t^{\omega} u - \nu \Delta u = f(x,t) \quad \forall\ (x,t) \in Q_T := \Omega \times (0,T],\\
&u|_{\partial\Omega} = 0 \quad \text{for } t \in (0,T],\\
&u(x,0) = u_0(x) \quad \text{for } x \in \Omega,
\end{aligned}$$

where $\Omega \subset \mathbb{R}^d$ $(d = 1,2,3)$, $\nu > 0$ is a constant diffusion coefficient, Δ is the Laplacian operator, and $f \in C(\overline{Q_T})$ with $\overline{Q_T} := \Omega \times [0,T]$. Here, $\mathcal{D}_t^{\omega} u$ represents the distributed order fractional derivative defined by

$$\mathcal{D}_t^{\omega} u(x,t) = \int_0^{\beta} \omega(\alpha) D_t^{\alpha} u(x,t)\, d\alpha, \quad 0 < \beta \leq 1,$$

where $\omega(\alpha) \geq 0$, $\displaystyle\int_0^{\beta} \omega(\alpha) \mathrm{d}\alpha = a_0 > 0$, and $D_t^{\alpha} u,\ (\alpha \in (0,1])$ is the standard fractional Caputo derivative of u of order α defined by

$$D_t^{\alpha} u(x,t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \frac{\partial u(x,s)}{\partial s}\, ds, \quad t > 0.$$

The exact solutions of he distributed order time-fractional diffusion equation usually are not available or may involve some special functions such as Mittag-Leffler function and Wright function that are very difficult to compute exactly. Hence, one needs to construct an efficient numerical scheme to solve these problem numerically. In this work, we use the well-known L1 method on a graded time mesh to compensate for the weak singularity at the starting point for the discretization of time Caputo fractional derivative and a stabilizer-free weak Galerkin finite element method in space. Under suitable chosen grading constant, an optimal convergence rates in the temporal direction and in the spatial direction for both semi-discrete and fully-discrete schemes have been achieved.

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Minisymposium
Numerical Methods for Fractional-Derivative Differential Equations

A Method-of-lines Approach for Space-fractional Nonlinear PDEs

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In this talk we discuss a method-of-lines approach for the numerical solution of space-fractional PDE models in one space dimension. The method is based on the use of square roots of appropriate finite-difference matrices for the spatial differential operator in the model. As an example, we explore eigenvalues and eigenvectors of the skew-symmetric matrix $\pm D_3$ and its square roots. These results are applied to the left- and right fractional differentiation operator, and are extended to the fractional Laplacian in one space dimension. Results are compared with an $L2$-discretization of the fractional derivative, as defined in the form of a weakly singular differential-integral operator. We obtain numerical evidence for the equivalence with an approach obtained by taking the double square root of integer powers of the positive-definite matrix $-D_2$ for the ordinary Laplacian in one dimension. Furthermore, a stability constraint (CFL-condition) is derived for the case of the explicit-Euler method, when applied in the second step of the method-of-lines. Finally, we show several nonlinear PDEs applications of this approach, among others, the space-fractional advection-diffusion PDE, Burgers equation and travelling waves in the space-fractional Fisher equation.

MS8 - RECENT ADVANCES ON NUMERICAL METHODS FOR FUNCTIONAL EQUATIONS AND APPLICATIONS

Organizers: Concetta Laurita, Donatella Occorsio, Maria Grazia Russo

Approximation is a well-studied mathematical topic, both from analytical and numerical points of view. Many problems of computational science, statistics, and probability require linear or nonlinear approximation, integration, or optimization of functions of many variables. Tensor networks, neural networks, and deep neural networks are the new tools for approximation especially in high-dimensional spaces. In a nutshell, the aim of approximation is to replace a target function, with a simpler one easy to evaluate and work with. Classical and modern approaches to this field cover various interesting techniques for multidimensional data and big data, information, signals, images, and so on.

The aim of this mini-symposium is to discuss both numerical aspects and the application of multivariate approximation since, in spite of its long tradition, many are open new problems like, for example, how to choose appropriate sampling sets for a given situation so that computations become tractable and the information loss is minimal or within acceptable tolerance limits.

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Minisymposium
Recent advances on numerical methods for functional equations and applications

Generalized-Hypergeometric Solutions in the Context of Heun Equations

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The general Heun equation, from which many other equations originate, is the most general Fuchsian second-order linear differential equation having four regular singular points We show that a Fuchsian differential equation having five regular singular points admits solutions in terms of a single generalized hypergeometric function for infinitely many particular choices of equation parameters.

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Minisymposium
Recent advances on numerical methods for functional equations and applications

Adapted Numerical Methods for Reaction-Diffusion Problems

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Several areas of applied sciences require the use of reaction-diffusion Partial Differential Equations (PDEs) to model phenomena of interest, such as vegetation growth (Eigentler et al., 2019), material corrosion processes (Mai et al., 2016), solar cells production (Maldon et al., 2020). Such models are usually multiscale and characterized by large spatial domains and high stiffness. The knowledge of these characteristics, together with a-priori known properties of the model, e.g. positivity or presence of oscillations, is very useful when constructing a numerical method for the related solution.

In this talk, we show numerical techniques for the construction of efficient and strongly problem-oriented methods, which are stable, i.e. able to handle stiffness preserving the main properties of the solution even for large discretization steps [2]. In particular, we focus on the use of TASE (Time-Accurate and highly-Stable Explicit) operators (Calvo et al., 2021) to stabilize parallelizable explicit peer methods [1]. Numerical experiments confirming the efficiency of the derived methods in solving some reaction-diffusion systems of PDEs from applications are carried out [2, 3].

References

[1] D. Conte, G. Pagano, B. Paternoster, *Time-accurate and highly-stable explicit peer methods for stiff differential problems*, Commun. Nonlinear Sci. Numer. Simul., 2023.

[2] D. Conte, G. Pagano, B. Paternoster, *Nonstandard finite differences numerical methods for a vegetation reaction–diffusion model*, J. Comput. Appl. Math., 2023.

[3] D. Conte, G. Frasca-Caccia, *A MATLAB code for the computational solution of a phase field model for pitting corrosion*, Dolomites Res. Notes Approx., 2022.

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Minisymposium
Recent Advances on Numerical Methods for Functional Equations and Applications

Numerical Model for Data Railway Fusion: Diagnostic Applications

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Several Data analysis techniques such as regression analysis, time series analysis, classification, and data visualization can be employed to gain insights and actionable recommendations from railway data. In the context of railway data, vertical displacement refers to the change in elevation or height of specific points along the railway infrastructure. It is a measure of the vertical movement or offset of railway tracks, bridges, tunnels, or other structures relative to a reference point or surface. By continuously monitoring vertical displacement, railway operators can identify early signs of track settlement or structural changes, allowing them to take appropriate maintenance and repair actions. As known, the measurements obtained from individual sensors are prone to inherent errors and uncertainties. Consequently, relying solely on these measurements for directly calculating vertical displacement may result in inaccuracies and limitations. To overcome this challenge, sensor fusion techniques have been developed, utilizing sophisticated mathematical algorithms that integrate and combine measurements from multiple sensors to estimate vertical displacement with improved accuracy and reliability. This fusion process considers the specific characteristics of each sensor, such as measurement accuracy and possible biases. By properly modeling these factors, fusion algorithms can compensate for the limitations of individual sensors and improve the overall accuracy of the estimation. In this talk, we explore some numerical methods to provide valuable insights into the dynamic behavior of a moving object and railways system. Experimental results obtained through extensive testing and analysis demonstrate the efficacy and potential of these fusion methodologies for predictive data analytics.

References

[1] Cuomo, S., Michele, P., Pragliola, M. (2017). A computational scheme to predict dynamics in IoT systems by using particle filter. Concurr Comput, 29 (11).

[2] Briales, E., Urda, P., & Escalona, J. L. (2021). Track frame approach for heading and attitude estimation in operating railways using on-board MEMS sensor and encoder. Measurement, 184, 109898.

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Minisymposium
Recent Advances on Numerical Methods for Functional Equations and Applications

Enrichment Strategies of the Bernardi Raugel Finite Element

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The simplicial vector linear finite elements are commonly used for numerically solving the stationary Stokes equations. They are known, however, to suffer from severe shortcomings in application to more complicated situations. An enriched finite element, that overcomes the aforementioned drawbacks, was proposed and developed by Bernardi and Raugel. It can be regarded as an advanced and generalized version of the conventional simplicial vector linear finite element, and it has been employed in a wide range of practical engineering computation fields. It uses polynomials as enrichment functions. However, the intractable linear dependence issue is always encountered when this type of enrichment functions is employed. In line with previous researches, the main contribution of this work is to present a general strategy for enriching the simplicial vector linear finite element by non-polynomial enrichment functions. This enriched finite element is defined with respect to any simplex, and can be regarded as an extension of Bernardi and Raugel element. A key role is played by a characterization result, given in terms of the non-vanishing of a certain determinant, which provides necessary and sufficient conditions, on the enrichment functions and functionals, that guarantee the existence of families of such enriched elements. We show that the enriched basis functions admit a closed form representation in terms of enrichment functions and functionals.

References

[1] F. Dell'Accio, F. Di Tommaso, A. Guessab, F. Nudo *A unified enrichment approach of the standard three-node triangular element*, Applied Numerical Mathematics, 187 (2023), pp. 1–23.

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Minisymposium
Recent Advances on Numerical Methods for Functional Equations and Applications

A Nyström Method for Hammerstein Integral Equations on a Closed Interval

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The topic of the talk is the numerical approximation of nonlinear integral equations of the Hammerstein type, defined on the closed real interval $[-1, 1]$:

$$f(y) + \lambda \int_{-1}^{1} k(x, y)h(x, f(x))dx = g(y), \qquad y \in [-1, 1],$$

where $\lambda \in \mathbb{R}$, with $|\lambda| \leq 1$, g and k are known functions defined on $[-1, 1]$ and $[-1, 1]^2$, respectively, h is defined on $[-1, 1]^2$ and f is the unknown in $[-1, 1]$.

The Hammerstein integral equations appear in nonlinear physical phenomena such as electromagnetic fluid dynamics, reformulation of boundary value problems with a nonlinear boundary condition.

The most popular numerical methods for solving these equations are collocation, Galerkin and Nyström methods, based on piecewise polynomial approximation [1].

Here we propose a Nyström method based on the Legendre Gaussian rule. The nonlinear system, equivalent to the Nyström method, is solved by an iteration scheme (Newton's or Broyden's one).

References

[1] K.E. Atkinson, *A survey of numerical methods for solving nonlinear integral equations*, J. Integral Equations Appl. 4(1992) 15-46.

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Minisymposium
Recent advances on numerical methods for functional equations and applications

On Computing Modified Moments for Half-range Hermite and Pollaczek–Hermite Weights in Floating Point Arithmetic

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In this talk we consider the problem of computing two different kinds of integrals:

$$\int_{a_i}^{b_i} f(x)w_i(x)dx, \quad i = 1, 2,$$

where $w_1(x) = e^{-x^2}$, $a_1 = 0$, $b_1 = \infty$, and $w_2(x) = e^{-x^2-\frac{1}{x^2}}$, $a_2 = -\infty$, $b_2 = \infty$. Although $w_1(x)$ and $w_2(x)$ are both positive weights, the associated system of orthogonal polynomials is not known. Therefore, it is not possible to compute the nodes and weights of the corresponding Gaussian rules in the standard way.

We approximate the above integral by a product quadrature rule. For both weights, it is needed to compute the modified moments:

$$\mathcal{M}_\ell^{(i)} = \int_{a_i}^{b_i} \tilde{p}_\ell(x)w_i(x)dx, \qquad \ell = 0, 1, 2, \ldots, \ i = 1, 2.$$

For $i = 1$, i.e., the half–range Hermite weight, we consider the system of orthonormal Laguerre polynomials $\{\mathcal{L}_\ell(x)\}_{j=0}^{\infty}$ as $\{\tilde{p}_\ell(x)\}_{\ell=0}^{\infty}$. We will show that, given $n > 1$, the vector of modified moments $\left[\mathcal{M}_0^{(1)}, \mathcal{M}_1^{(1)}, \ldots, \mathcal{M}_n^{(1)}\right]^T$ belongs to the null–space of a totally nonnegative matrix. Therefore, these moments can be computed to high relative accuracy.

The case $i = 2$, i.e., the Pollaczek–Hermite weight, can be handled in a similar way, choosing the orthonormal Hermite polynomials $\{\mathcal{H}_\ell(x)\}_{j=0}^{\infty}$ as $\{\tilde{p}_\ell(x)\}_{\ell=0}^{\infty}$ for computing the corresponding modified moments.

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Minisymposium
Recent Advances on Numerical Methods for Functional Equations and Applications

On the Stability of Recurrence Relations Arising in Orthogonal Polynomials Frameworks

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In this talk we consider recurrence relations arising in different contexts and analyze their stability properties. In particular, we focus on recurrence relations for: classical orthogonal polynomials of a discrete variable, such as Krawtchouk, Meixner, and Hahn polynomials [1]; computation of modified moments for Pollaczek and half–range Hermite weights [2, 3]; evaluation of Bessel functions; computation of the Hilbert transform of Jacobi weights [1]. Two techniques are usually considered to evaluate recurrence relations: in a forward fashion, given the initial condition(s) [1]; in a backward fashion, starting from dummy inital condition(s).
These tecniques have been extensively studied [1]. Nevertheless, such approaches turn out to be unstable in some cases.

Here, we propose a new algorithm, based on linear algebra tools, able to evaluate, in most cases, the considered recurrence relations in a reliable way [2, 3].

References

[1] W. Gautschi, *Orthogonal Polynomials: Computation and Approximation*, Oxford University Press, 2004.

[2] T. Laudadio, N. Mastronardi, D. Occorsio, *Computing integrals with an exponential weight on the real axis in floating point arithmetic*, Applied Numerical Mathematics, to appear.

[3] T. Laudadio, N. Mastronardi, P. Van Dooren, *On computing modified moments for half-range Hermite weights*, Numerical Algorithms, to appear.

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Minisymposium
Recent Advances on Numerical Methods for Functional Equations and Applications

A Method for the Approximation of Hadamard Transforms on [-1,1]

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In this talk we propose a method to approximate the weighted Hadamard transform of a given function f

$$\mathcal{H}_1^w(f,t) = \Xint-_{-1}^{1} \frac{f(x)}{(x-t)^2} w(x)\,dx, \tag{12}$$

where $t \in (-1,1)$ and $w(x) = v^{\alpha,\beta}(x) = (1-x)^\alpha(1+x)^\beta,\ \alpha,\beta > 0$ is a Jacobi weight. The proposed method is obtained by means of a simultaneous approximation technique involving the extended Lagrange interpolation process (cf. [1]) based on the zeros of the polynomial $p_{m+1}(\tau)p_m(\overline{\tau})$, where $\{p_n(\tau)\}_n$ and $\{p_n(\overline{\tau})\}_n$ denote the orthonormal sequences w.r.t the weights $\tau = v^{\rho,\sigma}$ and $\overline{\tau} = v^{\rho+1,\sigma+1}$, $\rho,\sigma > -1$, respectively.
Moreover, we introduce a scheme that combines the product formula based on the zeros of $p_m(\tau)$ and a new extended product rule. Such scheme allows a significant reduction in the number of samples of the function f.
The numerical stability and the convergence of this combined scheme are proved in suitable weighted uniform spaces. Finally, some numerical tests are presented in order to highlight the efficiency of the combined scheme and to confirm the theoretical estimates.

References

[1] G. Criscuolo, G. Mastroianni, D. Occorsio, *Convergence of Extended Lagrange Interpolation*, Mathematics of Computation, 55(191) (1990), pp. 197–212.

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Minisymposium
Recent Advances on Numerical Methods for Functional Equations and Applications

On solving some CSIE by de la Vallée Poussin filtered approximation

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A numerical solution of Cauchy Singular Integral Equations with constant coefficients based on some non standard polynomial quasi–projection of de la Vallée Poussin type is proposed.

Such kind of approximation presents several advantages over classical Lagrange interpolation such as the uniform boundedness of the Lebesgue constants, the near best order of uniform convergence to any continuous function, and a strong reduction of Gibbs phenomenon [1].

These features are inherited by the proposed numerical method which is stable and convergent, and provides a near best polynomial approximation of the sought solution by solving a well conditioned linear system. The numerical tests confirm the theoretical error estimates and, in case of functions subject to Gibbs phenomenon, they show a better local approximation compared with analogous Lagrange projection methods [2].

References

[1] W. Themistoclakis. *Uniform approximation on* $[-1, 1]$ *via discrete de la Vallée Poussin means*, Numer. Algorithms, 60(4)(2012), pp. 593–612.

[2] M. C. De Bonis and G. Mastroianni., *Direct methods for CSIE in weighted Zygmund spaces with uniform norm*, Riv. Mat. Univ. Parma, 2 (2011), pp. 29–55.

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Minisymposium
Recent Advances on Numerical Methods for Functional Equations and Applications

Filtered Integration Rules for the Hilbert Transform on $(0, +\infty)$

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The main topic is the approximation of the Hilbert transform of a given function f

$$\mathcal{H}^w f(t) := \int_0^{+\infty} \frac{f(x)}{x-t} w(x)dx, \qquad w(x) = x^\alpha \mathrm{e}^{-x}, \qquad \alpha > -1 \tag{13}$$

by means of de la Vallée Poussin polynomial of f (shortly VP polynomial) based on the zeros of the $n-$th Laguerre polynomial $p_n(w)$ and depending on the additional parameter $m \in \mathbf{N}$, with $0 < m < n$. $V_n^m(w, f)$, differently from the Lagrange polynomial $L_n(w, f)$ interpolating f at the same nodes, does not interpolate f, but for suitable choices of m and under proper assumptions, provides a better pointwise approximation than $L_n(w, f)$ offers. By approximating the density function f in (13) by $V_n^m(w, f)$ and $L_n(w, f)$, two different product integration rules are obtained: VP-rule and L-rule, respectively. The latter is well known and widely studied.

Here we introduce the product VP rule, showing that for f presenting some "pathologies" (peaks, cusps, etc.) localized in isolated points, it provides a better performance than L-rules.

MS9 - RECENT PROBLEMS AND METHODS IN COMPUTATIONAL FINANCE

Organizers: Karel in't Hout, Carlos Vázquez Cendón

In this minisimposium, some recent advances in the mathematical methods and computational techniques to solve a variety of problems arising in quantitative finance will be presented. These advances are mainly related to the mathematical modelling, mathematical analysis of the models, different appropriate numerical methods to solve them and also efficient computational techniques. Among the addressed financial problems, there are some related to option pricing, valuation adjustments related to counterparty risk, insurance products valuation, climate risk, equilibrium under heterogeneous economic agents, etc. Mathematical models are formulated in terms of partial (integro-) differential equations, backward stochastic differential equations, expectations, etc. Numerical methods involve probabilistic techniques, finite differences and finite elements, Monte Carlo based techniques, Picard iterations for nonlinear models or deep and machine learning techniques, for example.

Minisymposium
Recent Problems and Methods in Computational Finance

Identifying the Number of Latent Factors of Stochastic Volatility Models

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We provide a procedure to identify the number of latent factors of stochastic volatility models. The methodology relies on the non-parametric Fourier estimation method introduced by [1] and applies to high-frequency data. Based on the Fourier analysis, we first estimate the latent volatility process and then the volatilities and covariances of the processes that are gradually identified, such as volatility of volatility and leverage. The analysis of the eigenvalues spectrum of the Gram matrix can reveal information about the actual number of factors driving the process at hand. We corroborate our analysis by numerical simulations on single and multi factor models. Finally, we apply our methodology to intraday prices from the S&P 500 index futures.

References

[1] P. Malliavin and M.E. Mancino, *Fourier series method for measurement of multivariate volatilities*. Finance and Stochastics, 4: 49–61, 2002.

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Minysimposium
Recent Problems and Methods in Computational Finance

XVA Modelling and Computing in a Multicurrency Setting

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In this talk, we propose appropriate models to compute the total valuation adjustments (XVA) related to the presence of counterparty risk in a multicurrency setting by means of dynamic hedging methodologies. Besides the stochastic evolution of the assets in the different currencies, the presence of stochastic intensities of default and the consideration of constant or stochastic exchange rates are assumed when computing the XVA associated to European options contracts. These models can be formulated in terms of linear or nonlinear parabolic partial differential equations (PDEs)or in terms of expectations.

When the number of stochastic factors is no greater than two, we propose a Lagrange-Galerkin scheme (based on the method of characteristics and the finite element method) for solving the PDEs, eventually combined with fixed point techniques for the nonlinear problems. For problems that include more than two underlying stochastic factors (assets, intensities of default, and/or stochastic FX rates),we propose the use of Monte Carlo simulations applied to the formulations based on expectations, combined with a Picard method and the more efficient Multilevel Picard iteration (MPI) scheme for the nonlinear cases. We apply these techniques to different options of European type that validate the performance of the models as well as the proposed numerical methods.

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Minisymposium
Recent Problems and Methods in Computational Finance

Efficient Likelihood Estimation with Wavelets

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We propose a maximum likelihood approach to estimate the parameters of a stochastic volatility (SV) model. The SV model can be seen as a state-space model, this is, a stochastic model in discrete-time which contains two sets of equations, the state equation and the observation equation. While the first describes the transition of a latent process in time, the second shows how an observer measures the latent process at each time period. We infer the properties of the latent variable by means of a filtering algorithm. The evaluation of the likelihood function is a time-consuming task that involves updating and prediction steps of the state variable, leading to the computation of complicated integrals. We calculate these integrals by means of Shannon wavelets, and compare the root mean square error (RMSE) of the estimation with state-of-the-art methods. The results show that the RSME is dramatically reduced with a short CPU time with the use of wavelets.

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Impact of Correlation between Interest Rates and Mortality Rates on the valuation of Various Life Insurance Products

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In this paper, we establish the expression of the best estimate of a zero-coupon survival bond when modelling the interest rates and the mortality rates with two Hull and White models correlated to each other, meaning that we relax the traditional assumption of independence between mortality risk and interest rate risk. We investigate the impact of the inclusion of correlation on the best estimate of usual life insurance contracts and study in which cases the non-taking into account of correlation can lead to a severe underestimation of the best estimate.

Minisymposium
Recent Problems and Methods in Computational Finance

A Deep Solver for BSDEs with Jumps

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The aim of this work is to propose an extension of the deep solver by Han, Jentzen, E (2018) to the case of forward backward stochastic differential equations (FBSDEs) with jumps. As in the aforementioned solver, starting from a discretized version of the FBSDE and parametrizing the (high dimensional) control processes by means of a family of artificial neural networks (ANNs), the FBSDE is viewed as model-based reinforcement learning problem and the ANN parameters are fitted so as to minimize a prescribed loss function. We take into account both finite and infinite jumpactivity by introducing, in the latter case, an approximation with finitely many jumps of the forward process. We successfully apply our algorithm to option pricing problems in low and high dimension and discuss the applicability in the context of counterparty credit risk.

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Minysimposium
Recent Problems and Methods in Computational Finance

Artificial Neural Networks with Chebyshev Polynomials in Option Pricing

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Pricing different types of options is a subject of interest in finance. Classical numerical methods such as finite difference, finite elements or spectral methods, have been successfully applied to solve pricing problems in low-dimensional cases. However, the mentioned numerical methods suffer from the curse of dimensionality. When working in high-dimensional spaces, or with several underlying stocks, they become inefficient, as the computational cost grows exponentially. Artificial Neural Networks are a good solution to overcome the limitations of the previous methods. In particular, the purpose of this work is to combine the benefits of Artificial Neural Networks with Chebyshev polynomial approximation properties. We will see that applying a Chebyshev polynomial expansion can improve convergence rates of Artificial Neural Networks, providing an interesting framework for option pricing.

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Recent Problems and Methods in Computational Finance

A New Deep Solution Algorithm for Fully Coupled FBSDEs

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In this paper, we propose a new deep learning algorithm, for fully coupled FBSDEs (Forward Backward Stochastic Differential Equations) that are originated from stochastic control problems. Our algorithm is a further extension of the existing Deep BSDE method. At the current stage, we provide convergence results in the setting of drift control, yet through several numerical examples, we show that our algorithm not only provides higher accuracy in drift control problems but also solves diffusion control problems.

This is joint work with Balint Negyesi and Cornelis Oosterlee.

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Recent Problems and Methods in Computational Finance

Efficient Numerical Valuation of European Options under the Two-asset Kou Jump-diffusion Model

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This contribution concerns the numerical solution of the two-dimensional time-dependent partial integro-differential equation (PIDE) that holds for the values of European-style options under the two-asset Kou jump-diffusion model. A main feature of this equation is the presence of a nonlocal double integral term. For its numerical evaluation, we extend a highly efficient algorithm derived by Toivanen [1] in the case of the one-dimensional Kou integral. The acquired algorithm for the two-dimensional Kou integral has optimal computational cost: the number of basic arithmetic operations is directly proportional to the number of spatial grid points in the semidiscretization. For the effective discretization in time, we study seven contemporary operator splitting schemes of the implicit-explicit (IMEX) and the alternating direction implicit (ADI) kind. All these schemes allow for a convenient, explicit treatment of the integral term. We analyze their (von Neumann) stability. By ample numerical experiments for put-on-the-average option values, the actual convergence behaviour as well as the mutual performance of the seven operator splitting schemes are investigated. Moreover, the Greeks Delta and Gamma are considered.[2]

References

[1] J. Toivanen, *Numerical valuation of European and American options under Kou's jump-diffusion model*, SIAM J. Sci. Comp., 2008.

[2] K. J. in 't Hout, P. Lamotte, *Efficient numerical valuation of European options under the two-asset Kou jump-diffusion model*, to appear in J. Comput. Finance, 2023.

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Equilibrium Problems with Heterogeneous Agents under Jump-diffusion Models

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In this talk, we assume rational expectations to pose general equilibrium models with heterogeneous firms, which can enter or exit the industry. We consider a general Ito process with jumps for agent productivity dynamics, extending our previous work without jumps [2]. A Hamilton-Jacobi-Bellman (HJB) formulation models the endogenous decision of firms to remain or leave the industry [1]. All firms that exit are immediately replaced by new ones, so that the probability density function of firms satisfies a Kolmogorov-Fokker-Planck (KFP) equation with source term. Due to the presence of jumps, these equations are associated with partial-integro differential operators. Equilibrium models are completed with the household problem formulation and feasibility conditions. For the numerical solution, we propose a Crank-Nicolson method for the time discretization and the Adams-Bashforth scheme for the explicit treatment of integral terms. Moreover, we use an augmented Lagrangian active set (ALAS) method, jointly with a finite difference discretization for the HJB formulation and an adequate finite difference discretization for the KFP problem. For the global equilibrium problem, we propose a Steffensen algorithm. Finally, numerical examples illustrate the performance of proposed numerical methodologies as well as the expected behaviour of economic variables.

References

[1] Y. Achdou, F. J. Buera, J. M. Lasry, P. L. Lions, B. Moll. Partial differential equation models in macroeconomics, *Philosophical Transactions of Royal Society A: Mathematical, Phisical and Engineering Sciences*, 372 (2028), 20130397, 2014.

[2] J. Ráfales, C. Vázquez. Equilibrium models with heterogeneous agents under rational expectations and its numerical solution, *Communications in Nonlinear Science and Numerical Simulation*, 96, 105673, 2021.

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Minisymposium
Recent Problems and Methods in Computational Finance

Approximate Option Pricing under Jump-diffusion Stochastic Volatility Models Based on a Hull and White Type Formula

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In [1], a Hull and White type formula, that is, a theoretical and exact decomposition of the price of a plain vanilla option, is used to obtain approximate prices of plain vanilla options under the Heston model. These ideas have subsequently been extended to different stochastic volatility models with and without jumps (see [2]) and the methodology for obtaining approximate prices has been improved, see [3]. Results for more complex models (rough volatility, hybrid, two-factor, infinite activity jumps) have recently been obtained, see [4] and [5]. The aim of the talk is to summarize this methodology and discuss its competitiveness in terms of accuracy and computational cost with other recent methodologies for approximating option prices.

References

[1] E. Alòs, R. De Santiago and J. Vives (2015): *Calibration of stochastic volatility models via second order approximation: the Heston case*. International Journal of Theoretical and Applied Finance 18 (6): 1550036 (31 pages).

[2] R. Merino, J. Pospísil, T. Sobotka and J. Vives (2018): *Decomposition formula for jump diffusion models*. International Journal of Theoretical and Applied Finance 21 (8).

[3] A. Gulisashvili, M. Lagunas, R. Merino and J. Vives (2020): *Higher order approximation of call option prices in stochastic volatility models*. Journal of Computational Finance 24 (1).

[4] Y. El-Khatib, Z. S. Makumbe, J. Vives (2023): *Approximate option pricing under a two factor Heston-Kou stochastic volatility*. Submitted to Computational Management Science.

[5] Y. El-Khatib, Z. S. Makumbe, J. Vives (2023): *Decomposition of the option pricing formula for infinite activity jump-diffusion stochastic volatility models*. Preprint.

MS10 - RECENT TRENDS IN NUMERICAL METHODS FOR EVOLUTIONARY PROBLEMS

Organizers: Sebastianno Boscarino, Giuseppe Izzo, Eleonora Messina, Jie Shen

21st IMACS World Congress *University of Rome 'La Sapienza', Italy*

Minisymposium
Recent Trends in Numerical Methods for Evolutionary Problems

Multiscale Constitutive Framework of Blood Flow: Modeling and Numerics

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The significant morphological and mechanical variability of vessels, which results in complicated fluid-structure interaction (FSI) mechanisms between vessel walls and blood flow, is one of the many issues associated with the numerical modeling of the human cardiovascular system [3]. Hence, one of the main relevant goals in this complex computational setting is to have an easily extensible model and an accurate, efficient and robust numerical method [1]. This talk discusses a very flexible multiscale constitutive framework for modeling 1D blood flow. It is shown that various blood propagation phenomena can be recovered by an appropriate selection of the scaling parameters of the model, which are connected to various characterizations of the FSI mechanism (whether elastic or viscoelastic). The problem is solved with a third-order accurate Implicit-Explicit Runge-Kutta Finite Volume method, which guarantees consistency of the scheme with the various asymptotic limits of the model without affecting the time step size due to the smallness of the scaling parameters [2].

References

[1] G. Bertaglia, V. Caleffi, A. Valiani, Modeling blood flow in viscoelastic vessels: the 1D augmented fluid–structure interaction system, *Comput. Meth. Appl. Mech. Eng.*, 360(C):112772, 2020.

[2] G. Bertaglia and L. Pareschi, Multiscale constitutive framework of 1D blood flow modeling: Asymptotic limits and numerical methods, *Multiscale Model. Simul.*, in press, 2023.

[3] F. Piccioli, G. Bertaglia, A. Valiani, V. Caleffi, Modeling blood flow in networks of viscoelastic vessels with the 1-D augmented fluid–structure interaction system, *J. Comput. Phys.*, 464:111364, 2022.

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Non Standard Methods for Volterra Integral Equations: a Case Study in Mathematical Epidemiology

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Volterra integral and integro-differential equations appear in several applied problems and represent a suitable mathematical model for describing the evolution of various significant biological phenomena. In this context, we propose a non-standard finite differences numerical method for a general class of integro-differential equations with the aim to preserve the main characteristics of the original system and to maintain accuracy throughout long-term simulations [2]. The non-standard finite difference techniques were originally introduced by Mickens in [3], representing a pioneering development in the application of such methods to systems of ordinary differential equations. Here we extend this approach to integro-differential problems and we focus on a case study in the field of mathematical epidemiology. Specifically, we introduce an age-of-infection model incorporating the effect of human behavior in the disease, we analyze the stability of the equilibria and compare the results obtained to the corresponding discrete ones [1].

References

[1] B. Buonomo, E. Messina, C. Panico, A. Vecchio, *Age-of-infection epidemic model including behavioral changes*, in preparation.

[2] E. Messina, M. Pezzella, A. Vecchio, *Nonlocal finite difference discretization of a class of renewal equation models for epidemics*, MBE 20(7), 2023.

[3] R.E. Mickens, *Nonstandard Finite Difference Model of Differential Equations*, World Scientific, Singapore, 1994.

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Structure Preserving Schemes for the Allen-Cahn Type Equations

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In comparison with the Cahn-Hilliard equation, the classic Allen-Cahn equa- tion satisfies the maximum bound principle (MBP) but fails to conserve the mass. Here, we report the MBP and corresponding numerical schemes for the Allen-Cahn equation with nonlocal constraint for the mass conservation. In extension, we discuss the convective Allen-Cahn equation case.

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Conservative and Efficient Numerical Simulation for Time-fractional Diffusion Problems

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The time fractional diffusion problems are naturally suitable to describe diffusion processes with memory, since the fractional derivative depends on the past history of the function. However, this dependence represents an issue in the numerical simulations, since the computational cost of evaluating the history term at each time step may be high. Another important issue concerns the preservation of qualitative properties of the analytical model, as for example the conservation laws.

In this talk, we propose to discretize a time-fractional diffusion problem in space by a classical finite difference scheme. Then, to avoid the approximation of the long tail of the solution of step-by-step methods, we adopt a spectral method along time, which is exponentially convergent for a suitable choice of the function basis. We examine the sufficient conditions to determine conservation laws of diffusion equations of arbitrary fractional order in time. We show that the proposed numerical scheme satisfy a discrete analogue of these conditions and thus has conservation laws that approximate the continuous ones. Finally, we extend the analysis on the preservation of conservation laws to multistep methods, such as the Grünwald-Leitnikov scheme.

References

[1] K. Burrage, A. Cardone, R. D'Ambrosio, B. Paternoster, *Numerical solution of time fractional diffusion systems*, Appl. Numer. Math. 116, 82-94 (2017).

[2] A. Cardone, G. Frasca Caccia, *Numerical conservation laws of time fractional diffusion PDEs*, Fract. Calc. Appl. Anal. 25, 1459-1483 (2022).

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Numerical Preservation of Monotonicity and Positivity of Time-stepping Methods

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Given a differential problem whose solutions have a given qualitative property, e.g. monotonicity or positivity, its numerical preservation is an important issue in order to obtain numerical solutions with physical sense. The Strong Stability Preserving (SSP) theory can be used to obtain time step restrictions to preserve these qualitative properties. However, it is well known that for many problems, the stepsize bounds obtained with this approach are not sharp. One of the reasons is that many odd problems, that usually do not arise in applications, are included in the class of problems considered in the SSP theory. Sharper stepsize restrictions can be obtained by taking into account some additional property of the differential problem. In this talk, we show some results on numerical preservation of monotonicity an positivity for some of problems.

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New Highly Stiff-stable Schemes for Linear and Nonlinear Parabolic Equations

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We construct a class of new highly stiff-stable schemes of orders two to five for linear and nonlinear parabolic equations based on Taylor expansions at time $t_{n+\beta}$ where $\beta > 1$ is a tunable parameter. We show that their numerical solutions are bounded unconditionally (resp. for sufficiently small time steps) for linear (resp. nonlinear) parabolic equations, and derive their optimal error estimates for a large class of nonlinear parabolic equations. We also present numerical results to show the advantages of the new schemes compared with the classical IMEX schemes based on Taylor expansions at time t_{n+1}.

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Unconditionally Positive and Conservative Modified Patankar Linear Multistep Methods

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A wide variety of mathematical models for real life problems are given in the form of positive and conservative Production-Destruction differential Systems (PDS) [1]. Patankar-type schemes are linearly implicit integrators for PDS, traditionally based on Runge-Kutta schemes and specifically designed to be unconditionally conservative and positive [2, 3, 4]. Here we extend the Patankar approach to linear multistep methods and prove that the resulting discretizations retain, with no conditions on the step size, the positivity of the solution and the linear invariant of the continuous-time system. Moreover, we provide results on arbitrarily high order of convergence achieved through an embedding technique for the Patankar weights denominators.

References

[1] U. an der Heiden, M.C. Mackey, *The dynamics of production and destruction: Analytic insight into complex behavior*, J. Math. Biol., 16 (1982), pp. 75–101.

[2] J. Huang, W. Zhao, C.W. Shu, *A Third-Order Unconditionally Positivity-Preserving Scheme for Production-Destruction Equations with Applications to Non-equilibrium Flows*, J. Sci. Comput., 79 (2019), pp. 1015–1056.

[3] S. Kopecz, A. Meister, *Unconditionally positive and conservative third order modified Patankar-Runge-Kutta discretizations of production-destruction systems*, Bit Numer. Math., 58 (2018), pp. 691–728.

[4] D. Torlo, P. Öffner, H. Ranocha, *Issues with positivity-preserving Patankar-type schemes*, Appl. Numer. Math., 182 (2022), pp. 117–147.

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Approximation of High-order PDEs by Hyperbolic Systems

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In recent years, various authors have proposed to approximate the solution of certain diffusion equations and dispersive nonlinear wave equations by systems of first-order hyperbolic PDEs. We review these ideas and present a general framework for such *hyperbolizations*. We show that the technique can be applied to a very wide range of high-order PDEs, with potential advantages for efficient numerical solution. We also show that care must be taken in order to ensure that the hyperbolic system has a stable dispersion relation that approximates the original system.

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Numerical Analysis and Simulation for Two-phase Incompressible Flows

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In this talk, we will first present several efficient and high-precision schemes for the two-phase incompressible flows. These schemes are linear, decoupled and only require solving a sequence of Poisson type equations at each time step. We carry out a rigorous error analysis for the first-order scheme, establishing optimal convergence rate for all relevant functions in different norms. Next we shall discuss the consistent splitting GSAV approach for the two-phase incompressible flows and carry out theoretical analysis.

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An Energetic Spectral Element in Time Method for Nonlinear Gradient Systems

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In this talk, we present a spectral element in time spectral method for nonlinear gradient systems with the phase-field equations as examples. Different from commonly-used spectral in time methods, which employ spectral Petrov-Galerkin or weighted Galerkin approximations, the presented method use a natural (energetic) variational Galerkin form that can maintain the volume conservation and energy dissipation property of the continuous dynamical system. Another advantage of this method is that superconvergence is achieved at special time points. We use a spectral extrapolation to treat the nonlinear term explicitly. The explicit method can be improved by a few Picard-type iterations to recover the superconvergence. Numerical experiments verify that the proposed method using elements of polynomials of degree three outperforms the 4th-order BDF scheme and the ETD-RK4 method. The latter two are known to have good performances in solving phase-field equations. In addition to the standard Allen-Cahn equation, we also applied the method to a conservative Allen-Cahn equation. We note that the application of this method is not limited to phase-field Allen-Cahn equations. It is suitable for solving general, large-scale nonlinear dynamical systems.

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A General Framework of Implicit High-order Schemes for Hyperbolic Systems

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This talk is concerned with the challenges of devising high-order implicit schemes for systems of hyperbolic conservation laws.

When solving hyperbolic systems, a source of difficulty is represented by stiff problems that occur when the speeds span different orders of magnitude. In this case, implicit schemes may become convenient because they require to choose a time step constrained by the CFL stability condition.

In contrast, implicit schemes are not constrained to the CFL condition and, thus, can be used to set up larger time step sizes. However, implicit methods may be more computationally expensive than explicit ones, since they require the solution of a system of equations, in general nonlinear, at each time step.

Here, we deal with an efficient formulation of implicit high-order finite volume schemes. Achieving high-order accuracy requires to employ non-linear space reconstructions to prevent spurious oscillations. The use of such space-limiting procedures introduces a source of non-linearity which becomes computationally challenging when using implicit schemes.

The novel idea is to use an implicit first order scheme to pre-compute the nonlinearities of the space-limiting procedure making the resulting implicit high-order scheme nonlinear just because of the non-linearity of the flux function. This approach is tailored to third order implicit approximation achieved by using a third order DIRK for the time integration and a third order CWENO reconstruction for the space discretization.

References

[1] Puppo, Semplice, Visconti. *Quinpi: integrating conservation laws with CWENO implicit methods*. Commun. Appl. Math. Comput., 2023.

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An Asymptotic Preserving, Parallel Class of Time Discretizations for Singularly Perturbed Equations

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In this talk, we present recent results on a class of predictor-corrector multiderivative schemes [1] and their application to singularly perturbed differential equations. It is shown that for a broad class of ODEs, this class of methods is asymptotically preserving under rather mild presentations. Subsequently, the application to the low-Mach Euler equations is discussed, also here, the AP property is discussed. Selected numerical results to underline and extend the theoretical aspects are given.

References

[1] J. Schütz, D. C. Seal, and J. Zeifang *Parallel-in-time high-order multiderivative IMEX methods*, Journal of Scientific Computing **90**(54) (2022).

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Explicit Runge-Kutta Schemes with Weak Stage Order and an Optimal Number of Stages

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Runge-Kutta (RK) methods may exhibit order reduction when applied to stiff problems. For linear problems with time-independent operators, order reduction can be avoided if the method satisfies certain weak stage order (WSO) conditions. WSO is less restrictive than traditional stage order conditions and compatible with an ERK or DIRK structure. This talk extends recently developed order barrier bounds [1, 2] to explicit RK schemes. The new barriers relate a schemes WSO to its classical order and number of stages. This bounds the fundamental accuracy of ERK methods applied to stiff problems. We devise (linear) SSP schemes with optimal WSO, demonstrate their efficacy on a suite of test cases, and characterize several features of the resulting schemes. The key mathematical ideas make use of RK irreducibility, pairs of orthogonal invariant subspaces and a "hidden" Sylvester equation in the RK WSO conditions.

References

[1] A. Biswas, D. Ketcheson, B. Seibold, D. Shirokoff *Design of DIRK schemes with high weak stage*, Comm. App. Math. Comp. Sci., 18:1–28 (2023).

[2] A. Biswas, D. Ketcheson, B. Seibold, D. Shirokoff *Algebraic structure of the weak stage order conditions for Runge-Kutta methods*, (2023).

MS11 - RECENT TRENDS ON NUMERICS OF SINGULARLY PERTURBED DIFFERENTIAL EQUATIONS

Organizer: Natesan Srinivasan

Singularly perturbed differential equations arise in various areas of science and engineering, including fluid dynamics, elasticity, chemical reactor theory, etc. It is too difficult to obtain the numerical approximate solutions of these problems by using classical finite difference, finite element, and finite volume methods, because of the presence of boundary layers. Devising efficient numerical methods to solve singularly perturbed differential equations is one of the big challenges and it has attracted several researchers for the past few decades.

The main idea of this mini-symposium is to provide a platform to the researchers working in this area to share their latest research contributions and to discuss the future directions towards solving these problems.

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Recent Trends on Numerics of Singularly Perturbed Differential Equations

Fractal Quintic Spline Solutions for Singularly Perturbed Boundary-value Problems

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A fractal quintic spline is used to get the numerical solutions for the following singularly perturbed boundary-value problems.

$$\left.\begin{aligned} -\varepsilon u''(x) + p\, u(x) = f(x), \quad x \in (0,1), \\ u(0) = \eta_0, \quad u(1) = \eta_1, \end{aligned}\right\}$$

where $p > 0$, $f(x)$ is sufficiently smooth function in $[0,1]$ and $0 < \varepsilon \leq 1$. Error analysis of the proposed method is carried out and it tells that the proposed method has fourth-order convergence. Further, numerical examples are provided to validate our theoretical results.

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Recent Trends on Numerics of Singularly Perturbed Differential Equations

An Efficient Uniformly Convergent Method for Two Dimensional Parabolic Convection-diffusion Singularly Perturbed Systems

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In this work we consider the numerical approximation of the exact solution of initial and boundary value problems associated to coupled 2D parabolic singularly perturbed systems of convection diffusion type, when the coupling is produced by the reaction terms. Such problems are given by

$$\begin{cases} \mathcal{L}_\varepsilon(t)\mathbf{u} \equiv \dfrac{\partial \mathbf{u}}{\partial t}(\mathbf{x},t) + \mathcal{L}_{\mathbf{x},\varepsilon}(t)\mathbf{u}(\mathbf{x},t) = \mathbf{f}(\mathbf{x},t),\ (\mathbf{x},t) \in Q \equiv \Omega \times (0,T], \\ \mathbf{u}(\mathbf{x},t) = \mathbf{g}(\mathbf{x},t),\ (\mathbf{x},t) \in \partial\Omega \times [0,T],\ \mathbf{u}(\mathbf{x},0) = \varphi(\mathbf{x}),\ \mathbf{x} \in \Omega, \end{cases} \tag{14}$$

where $\Omega = (0,1)^2$, $\mathbf{x} = (x,y)^T$ and the spatial differential operator $\mathcal{L}_{\mathbf{x},\varepsilon}(t)$ is defined as

$$\mathcal{L}_{\mathbf{x},\varepsilon}(t)\mathbf{u} \equiv -\mathcal{D}\Delta\mathbf{u} + \mathcal{B}_1(\mathbf{x})\frac{\partial \mathbf{u}}{\partial x}(\mathbf{x},t) + \mathcal{B}_2(\mathbf{x})\frac{\partial \mathbf{u}}{\partial y}(\mathbf{x},t) + \mathcal{A}(\mathbf{x},t)\mathbf{u}, \tag{15}$$

being $\mathcal{D} = \mathrm{diag}(\varepsilon_1, \varepsilon_2)$ the diffusion matrix. We assume that the convection matrices $\mathcal{B}_k, k = 1,2$ are diagonal, the reaction matrix $\mathcal{A}$ is a full M-matrix and the diffusion parameters ε_1 and ε_2 can be very small, satisfying $0 < \varepsilon_2 \leq \varepsilon_1 \ll 1$.

In general, when the diffusion parameters at both equations have a different order of magnitude, overlapping regular boundary layers appear at the outflow boundary of the spatial domain. The numerical method used to solve the continuous problem combines the classical upwind scheme, to discretize the spatial variables on an adequate nonuniform mesh of Shishkin type, and the standard fractional implicit Euler method joint to a splitting of the discrete differential operator by directions and components to integrate in time. Using this technique, we obtain a uniformly convergent method, which has first order in time and almost first order in space. Such method requires to solve only tridiagonal linear systems to obtain the numerical solution; consequently, the computational cost of this method is considerably smaller than the corresponding one to standard implicit methods which have been considered previously in the literature. Moreover, the advantages of our proposal increase when the number of equations in the system grows. The numerical results obtained for some test problems corroborate in practice the good behavior and the advantages of the constructed method.

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Low-degree Robust Finite Element Scheme for Inhomogeneous Fourth Order Perturbation Problem

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This talk is concerned with the inhomogeneous fourth order perturbation problem

$$\varepsilon^2\Delta(\sigma\Delta)u - \Delta u = f \tag{16}$$

where $0 < \varepsilon \ll 1$ is a small perturbation parameter and σ is a varying coefficient. Due to the inhomogeneous essence of σ, the standard integration-by-part technique does not apply, and general schemes which work for the perturbation problem $\varepsilon^2\Delta^2 u - \Delta u = f$ do not simply work, particularly the ones based on nonconforming (thus low-degree) finite elements for H^2 problems.

In this talk, low-degree robust finite element schemes for the model problem (16) will be introduced. The key ingredient is an identity of the form

$$\sum_{T\in\mathcal{T}_h}\int_T \nabla^2 w_h \nabla^2 v_h = \sum_{T\in\mathcal{T}_h}\int_T \Delta w_h \Delta v_h \tag{17}$$

for certain finite element functions w_h and v_h. The identity (17) can be viewed as a discrete strengthened Miranda-Talenti estimate which plays important roles in many applications. Some specific finite element schemes with (17) holding and thus working for (16) are presented, including particularly a finite element scheme with piecewise quadratic polynomials, thus of lowest degree. Some relevant further applications of these finite element functions are also given.

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A Direct Discontinuous Galerkin Finite Element Method for Two Parameter Singular Perturbation Problems

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The singular perturbation problem is a challenging mathematical phenomenon that occurs when a differential equation exhibits rapidly changing behavior in certain regions of the domain. In this study, we propose a novel approach to tackle the singular perturbation problem using the Direct Discontinuous Galerkin (DDG) method. DDG method is applied for numerical approximation of two-parameter singularly perturbed parabolic problems. We applied fully discrete scheme that is backward Euler method for time and DDG method for space variable. We have shown that method is stable and of the optimal order of convergence. Numerical results are given to verify our theoretical findings.

References

[1] H. Liu and J. Yan. The direct discontinuous galerkin (ddg) method for diffusion with interface corrections, Communications in Computational Physics, 8(3):541–554, 2010.

[2] J. Cheng, X. Yang, X. Liu, T. Liu and H. Luo. A direct discontinuous galerkin method for the compressible navier–stokes equations on arbitrary grids, Journal of Computational Physics, 327:484–502, 2016.

[3] G. Singh and S. Natesan. Superconvergence properties of discontinuous Galerkin time stepping for singularly perturbed parabolic problems. *Numer. Algorithms.*, 90:1073-1090, 2022.

[4] G. Singh and S. Natesan. Study of the NIPG method for two-parameter singular perturbation problems on several layer adapted grids. *J. Appl. Math. Comput.*, 63(1–2):683-705, 2020.

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A Novel Fully-Implicit FMM for 2D Singularly Perturbed Semilinear Parabolic PDEs with Non-homogeneous Boundary Data

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This article aims to develop and analyze an efficient higher-order numerical approximation for two-dimensional singularly perturbed semilinear parabolic convection-diffusion problems with non-homogeneous time-dependent boundary data. To achieve the aim, we approximate the governing nonlinear problem by developing a fully-implicit fitted mesh method (FMM) followed by the extrapolation technique. The method uses the fractional-step implicit-Euler method for the temporal discretization with an appropriate evaluation of the boundary data. The spatial discretization is based on a hybrid finite difference scheme. To accomplish this, an appropriate non-uniform rectangular mesh is used for discretizing the spatial domain, and an equidistant mesh is used for discretizing the time domain. At first, we study stability and asymptotic behavior of the analytical solution of the governing nonlinear problem. We then discuss stability of the fully-implicit method and establish ε-uniform convergence result in the supremum-norm. Thereafter, we analyze the Richardson extrapolation technique solely for the time variable to improve the order of convergence in the temporal direction. Finally, numerical results are presented to support the theoretical findings.

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Parameter-robust Numerical Analysis of a Numerical Scheme for a Parabolic Reaction-diffusion Equation with Time Delay Having Interior and Boundary Layers in its Solution

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In this article, we are interested in the parameter-robust numerical analysis of a reaction-diffusion delay differential equation having an interface in its domain. A special case where the diffusion coefficient is a small positive parameter is considered. The source term in the equation can have discontinuities along the interface. The problem's solution exhibits interior and boundary layers as the parameter approaches zero; which makes the problem challenging in establishing the parameter-robust convergence of any applied classical numerical techniques with respect to the parameter. The domain is discretized using a non-uniform mesh. The problem is discretized using a central difference scheme for the mesh points not on the interface and a special upwind central difference scheme for the mesh points on the interface. The solution and its numerical analog are decomposed into regular and singular components. Some appropriate a priori bounds on derivatives of the exact solution's regular and singular components have been given. Using these bounds, the parameter-robust convergence of the scheme is proved. Finally, numerical experiments are conducted to verify the method's efficiency and parameter robustness.

Keywords

Singularly perturbed, parabolic problems, time-delay, reaction-diffusion, interface problem, interior and boundary layers, parameter-robust convergence.

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Recent Trends on Numerics of Singularly Perturbed Differential Equations

Efficient Finite Element Method for 2D Parabolic Convection Diffusion Problems with Discontinuous Source Term

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This article deals with a class of 2D parabolic singularly perturbed convection diffusion problems with a special interior line source. An operator splitting method with streamline diffusion finite element method is suggested [1, 2, 3, 4]. It is proved that the present method is converges uniformly with respect to the parameter. Numerical illustrating examples will be provided.

References

[1] S. Ganesan, An operator-splitting Galerkin/SUPG finite element method for population balance equations: stability and convergence, ESAIM Math. Model. Numer. Anal. 46 (2012) 1447–1465.

[2] A. Das, S. Natesan, Higher-order convergence with fractional-step method for singularly perturbed 2D parabolic convection-diffusion problems on Shishkin mesh, Comput. Math. Appl. 75 (2018) 2387–2403. https://doi.org/10.3390/math11092034

[3] D. Avijit, S. Natesan, A novel two-step streamline-diffusion FEM for singularly perturbed 2D parabolic PDEs,Applied Numerical Mathematics 172 (2022) 259–278

[4] R. Soundararajan, V. Subburayan, Patricia J. Y. Wong, Streamline Diffusion Finite Element Method for Singularly Perturbed 1D-Parabolic Convection Diffusion Differential Equations with Line Discontinuous Source, Mathematics 2023, 11(9), 2034;

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Richardson Extrapolation Technique for Singularly Perturbed Degenerate Parabolic PDEs with Two Parameters

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Abstract

Here, we propose a numerical scheme to solve singularly perturbed two-parameter degenerate parabolic PDEs of convection-diffusion type. In order to discretize the domain, we use uniform meshes in the time-direction and layer-adapted piecewise-uniform meshes in the spatial domain. To discretize the PDE, we use the implicit-Euler scheme for the time derivative and classical finite difference scheme for the spatial derivatives. The proposed numerical scheme is first-order convergence in both time and spatial variables. Stability and parameter-uniform error estimates are obtained. Further, to enhance the order of convergence, here, we apply the Richardson extrapolation technique, which produces second-order convergence. The theoretical error estimates are validated by some numerical examples.

Keywords

Singularly perturbed two-parameter parabolic PDEs, boundary layers, layer-adapted nonuniform meshes, uniform convergence, Richardson extrapolation technique.

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Recent Trends on Numerics of Singularly Perturbed Differential Equations

The local discontinuous Galerkin method for two singularly perturbed convection-diffusion problems with exponential and characteristic layers

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In [1, 2] the local discontinuous Galerkin (LDG) finite element method is used to solve two convection-diffusion problems posed on the unit square in $\mathbb{R}^2$. The solution of [1] has exponential boundary layers on two sides of the square, while that of [2] has one exponential boundary layer and two characteristic (parabolic) boundary layers. For each problem, tensor-product piecewise polynomials of degree $k > 0$ are analysed on three families of layer-adapted meshes: Shishkin-type, Bakhvalov-Shishkin-type and Bakhvalov-type. Energy-norm supercloseness results for both problems, using a local Gauss-Radau projection of the true solution into the finite element space, imply new optimal L^2 convergence results for the error in the computed solution. Furthermore, in [2] we establish the first uniform convergence result for the LDG method applied to a problem with characteristic boundary layers. Numerical experiments in [1, 2] demonstrate the sharpness of all our theoretical results.

References

[1] Y. Cheng & M. Stynes, *Supercloseness of the local discontinuous Galerkin method for a singularly perturbed convection-diffusion problem*, Math. Comp. 92 (2023), pp.2065–2095.

[2] Y. Cheng & M. Stynes, *The local discontinuous Galerkin method for a singularly perturbed convection-diffusion problem with characteristic and exponential layers*, Numer. Math. (to appear).

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Recent Trends in Numerics of Singularly Perturbed Differential Equations

A Weak Galerkin Method for a Third-order Singularly Perturbed Reaction-diffusion Problem

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We apply a weak Galerkin finite element method (WG-FEM) for solving the following third-order singularly perturbed reaction–diffusion problem

$$\varepsilon^2 u'''(x) - b(x)u'(x) + c(x)u(x) = f(x) \quad \text{in } \Omega = (0,1), \tag{18}$$

$$u(0) = u(1) = u'(1) = 0, \tag{19}$$

where $0 \leq \varepsilon \ll 1$ is the perturbation parameter. Assume that $b(x) \geq \beta^2 > 0, \quad c(x) + \frac{1}{2}b'(x) \geq \gamma > 0, \quad x \in \Omega$, for some constant $\beta, \gamma > 0$. The WG-FEM which uses discontinuous test and trial functions has been introduced for the first time in [1] for solving second order elliptic partial differential equations. The method has been applied to singularly perturbed convection-diffusion problems in 1D and in 2D. It has been further applied to biharmonic problems on polytopal meshes in [2]. However, there is no result on the WG-FEM for the third-order singularly perturbed reaction-diffusion problem using layer-adapted meshes. Our goal is to fill this gap in the literature. We prove almost optimal uniform convergence in the energy-like norm, uniformly in the singular perturbation parameter on the layer-adapted meshes. These layer-adapted mesh will include Shishkin meshes, Bakhvalov–Shishkin meshes, and a Bakhvalov-type meshes. The theoretical findings are supported by some numerical examples. These numerical experiments show that the sharpness of our results.

References

[1] J. Wang, X. Ye, *A weak Galerkin finite element method for second-order elliptic problems*, Journal of Computational and Applied Mathematics 241 (2013) 103–11.

[2] L. Mu, J. Wang, X. Ye, *Weak Galerkin finite element methods for the biharmonic equation on polytopal meshes*, Numer. Methods Partial Differential Equations 30 (3) (2014) 1003–1029.

MS12 - SINGLE-SCALE AND MULTI-SCALE MODELLING: APPLICATIONS TO ECOLOGY, CELL BIOLOGY AND MEDICINE

Organizers: Raluca Eftimie, Zeina Masry, Antoine Perasso, Ezio Venturino

The advances in various technologies over the past few years have led to the collection of an enormous amount of data in ecology, cell biology and medicine: from the behaviour of cells and molecules (in the context of health and disease), to the behaviour of animals and their interactions with the environment. To make sense of this data, and to understand the complex biological and ecological processes associated with this data, researchers have been using a variety of approaches: from deterministic and stochastic modelling approaches combined with numerical simulations, to artificial intelligence approaches. This event will bring together researchers focusing on mathematical and statistical modelling of various biological, ecological and medical phenomena, with the goal of summarising some of the recent advances in the field and discussing the new open problems.

Minisymposium
Single Scale and Multi-scale Modelling:
Applications to Ecology, Cell Biology and Medicine

Enhanced Forecasting of Biomass-toxicity-water Models Using Numerical Simulations

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Plant-soil feedback plays a fundamental role, by shaping nutrient availability, altering soil properties, influencing plant interactions, and engaging in mutualistic relationships with soil microorganisms, in the emergence of vegetation patterns. It is essential to understand these feedback processes in order to manage and conserve ecosystems, predict responses to environmental change, and implement appropriate land management strategies. The formation of vegetation patterns has been the focus of significant study and debate over the years, and it has been linked to two main mechanisms: the depletion of water in the center of vegetation patches and the production of toxicity by litter decomposition in soil. In this study, we investigate the role of water depletion and autotoxicity in the formation of spatial patterns. We compare various reaction-diffusion PDE models that describe the dynamics of plant biomass under water scarcity and the presence of toxicity caused by the decomposition of litter. We incorporated logistic and exponential growth functions to capture different growth patterns, along with mortality and inhibitor terms to simulate the component's individual death rates and inhibitory effects. Using appropriate numerical techniques, we solved six alternative reaction-diffusion PDE models that we proposed, and MATLAB was used for the simulations.

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A New Numerical Solution for an Age-structured Population Model with Infinite Life Span

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The choice of the age as a physiological parameter to structure a population and describe its dynamics involves the election of the life-span. An unbounded life-span is useful, not only new models appears in this framework, but also it is required by the study of the stability of equilibria. Its numerical integration is usually perform with bounded domains. However, we propose a new numerical method which employs the unbounded domain. It is completely analysed and second order of convergence is established. We report some numerical experiments to show numerically the results

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Phenotype Divergence and Cooperation in Isogenic Multicellularity and in Cancer

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We discuss the mathematical modelling of two of the main mechanisms which pushed forward the emergence of multicellularity: phenotype divergence in cell differentiation, and between-cell cooperation. In line with the atavistic theory of cancer, a disease that is specific of multicellular animals, we set special emphasis on how both mechanisms appear to be reversed, however not totally impaired, rather hijacked, in tumour cell populations. Two settings are considered: the completely innovating, tinkering, situation of the evolutionary emergence of multicellularity, which we assume to be constrained by external pressure on the cell populations, and the completely planned - in the *body plan* - situation of the physiological construction of a developing multicellular animal from the zygote (fecundated egg), or of bet hedging in tumours, assumed to be of clonal formation, although the body plan is largely - but not completely - lost in its constituting cells. We show how cancer impacts these two settings and we sketch mathematical models for them. We present here our contribution to the question at stake with a background from biology, from mathematics, and from philosophy of science.

References

[1] Alvarez, F.E. & Clairambault, J. (2023). Phenotype divergence and cooperation in isogenic multicellularity and in cancer: a mathematical and philosophical contribution. *In preparation.*

[2] Alvarez, F.E., Carrillo, J.A., & Clairambault, J. (2022). Evolution of a structured cell population endowed with plasticity of traits under constraints on and between the traits. *J. Math. Biol.* 85:64.

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Stochastic Modeling of Biological Oscillations: the Circadian Rhythm Model

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Shedding light on the oscillatory mechanisms occurring in some relevant complex biochemical processes is an intriguing challenge. Here we focus on such a topic by modeling, with a stochastic approach, the biological process of the circadian clock. In almost all living organisms, countless molecules synchronize their dynamic behavior to produce periodic oscillations observable at the macroscopic level, with a period close to 24 hours. The main biochemical process from which these oscillations originate is the negative self-regulation exerted by the so-called *clock protein* on the expression of its gene [1]. In this framework, in a previous work [2] we proposed a stochastic model governed by Chemical Master Equations (CMEs). In this talk, we provide a possible extension of the stochastic approach by using stochastic differential equations (SDEs) which, on the one hand, overcome the curse of the dimensionality of the discrete-state CME approach and, on the other hand, preserve (by means of an approximate formulation) the stochastic nature of the phenomenon under study.

References

[1] A. Goldbeter, *A model for circadian oscillations in the Drosophila period protein (PER)*, Proc. R. Soc. London Ser. B, 261 (1995), pp. 319—324.

[2] G. Mavelli, A. Borri, P. Palumbo, A. M. Bersani, *On the qualitative behaviour of oscillating biochemical systems: the stochastic approach*, in: Problems in Mathematical Biophysics, SEMA SIMAI Springer Series, volume in memory of Alberto Gandolfi, (d'Onofrio, A. Fasano, F. Papa, C. Sinisgalli), Springer, 2023 (to appear).

Minisymposium
Single-scale and Multi-scale Modelling:
Applications to Ecology, Cell Biology and Medicine

Evolution of Populations Structured by Dietary Diversity and Starvation: Cross-diffusion Systems

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Cross-diffusion systems are nonlinear parabolic systems that model the evolution of densities or concentrations of multicomponent populations in interaction.

In this talk, we study the evolutionary dynamics of two species in competition, modeled by a triangular cross-diffusion system driven by dietary diversity. More precisely, we show the existence of weak solutions by rigorously proving the passage from an approximating Lotka-Volterra reaction-diffusion system with linear diffusion, towards a cross-diffusion system at the fast reaction limit. The resulting limit gives a cross-diffusion system of starvation-driven type. The main tools used to pass the limit rigorously consist of a priori estimates, given by the analysis of an entropy functional, and compactness arguments. This work is based on [1].

References

[1] E. Brocchieri, L. Corrias, H. Dietert, Y.J. Kim Evolution of dietary diversity and a starvation driven cross-diffusion system as its singular limit, J. Math.Biol. 83, 58 (2021).

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Minisymposium
Single scale and multi-scale modelling:
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Modeling Metastatic Tumor Evolution, Numerical Resolution and Growth Prediction

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In this talk I will present the work developed in [1], where we have introduced a generalized metastatic tumor growth model that describes the primary tumor growth by means of an Ordinary Differential Equation (ODE) and the evolution of the metastatic density using a transport Partial Differential Equation (PDE), [3]. The numerical method is based on the resolution of a linear Volterra integral equation (VIE) of the second kind, which arises from the reformulation of the ODE-PDE model, [2]. The convergence of the method is proved and error estimates are given. The computation of the approximate solution leads to solve well conditioned linear systems. Here we focus our attention on two different case studies: lung and breast cancer. We assume five different tumor growth laws, for each of them, different metastatic emission rates between primary and secondary tumors, and last that the new born metastases can be formed by clusters of several cells.

References

[1] Bulai IM, De Bonis MC, Laurita C, Sagaria V (2022). *Modeling metastatic tumor evolution, numerical resolution and growth prediction*, Mathematics and Computers in Simulation 721–740.

[2] Hartung N. (2015). *Efficient resolution of metastatic tumor growth models by reformulation into integral equations.* Discrete and Continuous Dynamical Systems - Series B 20(2):445-467.

[3] Iwata K, Kawasaki K, Shigesada N. (2000). *A dynamical model for the growth and size distribution of multiple metastatic tumors.* J Theor Biol.

Joint work with: Maria Carmela De Bonis, Concetta Laurita and Valeria Sagaria

Minisymposium
Single scale and multi-scale modelling:
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Fractional Diffusive Fisher Equation

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We discuss the solution of various generalized forms of (Fisher) Diffusion Equations, which plays an important role in the study of heat and mass transfer and in biology and ecology, for population diffusion. We use different tools ranging from the use of Hermite-Kampé de Fériet polynomials of higher and fractional order to operational techniques. We show that these methods are useful to obtain both numerical and analytical solutions.

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Blood Sample Based Early Cancer Detection Using Conformal Prediction

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Our work aims at developing a method for early detection of malignant cancer cells based on analysing blood samples. Our main contribution is a novel procedure based on testing for the presence of a malignant tumor using a model of tumour growth and protein shedding recently proposed in [2].

Since the likelihood ratio test only works when identifiability of the model parameters under the null hypothesis holds, we show that it is not applicable in the present setup. We therefore propose an alternative approach based on a recent statistical procedure introduced by Algeri et al. in [1].

In a second stage, we complement the proposed testing procedure with a new "conformal prediction"-based approach in order to control the error rate, following the lines of [3]. The conformalised methodology is shown to provide stronger confidence when dealing with potential model misspecification.

References

[1] Algeri, S. and van Dyk, D.A., 2020. Testing one hypothesis multiple times: The multidimensional case. Journal of Computational and Graphical Statistics, 29(2), pp.358-371.

[2] Avanzini, S., Kurtz, D.M., Chabon, J.J., Moding, E.J., Hori, S.S., Gambhir, S.S., Alizadeh, A.A., Diehn, M. and Reiter, J.G., 2020. A mathematical model of ctDNA shedding predicts tumor detection size. Science advances, 6(50), p.eabc4308.

[3] Bates, S., Angelopoulos, A., Lei, L., Malik, J. and Jordan, M., 2021. Distribution-free, risk-controlling prediction sets. Journal of the ACM (JACM), 68(6), pp.1-34.

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Modelling Inflammation in Cancer and Wound Healing: Single-scale and Multi-scale Approaches

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The relation between cancer and wound healing has been recognized for a long time. Some of the inflammatory mechanisms that regulate wound healing (e.g., via macrophages and fibroblasts) were also shown to promote the growth of malignant cancers. One cell population important for both the evolution of cancers and wound healing process is the macrophage. This cell population is very heterogeneous, with the extreme phenotypes described by (i) the pro-inflammatory and anti-tumour M1 cells; and (ii) the anti-inflammatory and pro-tumour M2 cells. The cytokines and growth factors in the micro-environment have an important role on the macrophage polarity (i.e., differentiation towards M1-like cells or M2-like cells), and the transitions between different phenotypes.

In this presentation we overview some single-scale and multi-scale mathematical models we developed over the last few years to describe the role of macrophages in cancers and wound healing: from single-scale ODEs and PDEs, to multi-scale integro-differential models and partial integro-differential equations. For all these different mathematical models we present and discuss numerical simulations. We also discuss parameter identification for single-scale models and multi-scale models.

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Modelling and Investigating Memory Immune Response in Acute SARS-CoV-2 Reinfection.

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Understanding effector and memory immune responses against SARS-CoV-2 infections is extremely important in the control of these infections. In this study, we investigate the role of memory cells in the immune response against acute SARS-CoV-2 reinfection with the help of within-host mathematical models. To this end, we adapt a previously published within-host model [1] that describes the immune response against the SARS-CoV-2 by including two types of memory cells, memory $CD8^+$-T cells and memory B-cells. We investigate the model by identifying the virus-free steady states and the virus-present steady states and study their stabilities. Since this first model could not display a steady state for healthy cells that would include also memory cells we then propose a second reduced model, which allows us to obtain a stable healthy steady state with memory cells. Finally, sensitivity analysis for both models leads to an identification of memory-related parameters that are most important for model outcome. Overall, this study shows that an healthy steady state characterised by the presence of memory cells can be achieved after acute reinfection with SARS-CoV-2 if the immune system adapts to the severity of the damage.

References

[1] S. Mehrshad, A. Layton *LModeling within-host SARS-CoV-2 infection dynamics and potential treatments*, Viruses, 2021.

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Minisymposium
Single Scale and Multi-scale Modelling:
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Modelling Plant-nematodes Interactions to Understand Plant Tolerance

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Root-knot nematodes (RKN) of the genus Meloidogyne spp. cause considerable yield losses in numerous crops worldwide. The dynamics and outcomes of crop–pest interactions depend on the ecological conditions, including the phenotypes of the interacting species, their physiology and the abiotic environment. In theoretical ecology, most mathematical models that describe these interactions either focus on plant physiology and do not consider pest dynamics, or conversely are based on the pest life cycle but neglect plant physiology and defense response. We are particularly interested in understanding the mechanisms that underlie plant tolerance, that is the ability of plants to sustain RKN infestation with limited yield losses.

To address this, we built a mechanistic model of plant–RKN interactions that explicitly couples plant physiology and pest demography, including both the known effect of pests on crop and crop on pests. Based on a mechanistic description of resource acquisition and transport, the plant model represents both vegetative and reproductive phase. The RKN model includes the free-living larval stage and the nematode development stages within the plant root. The model was calibrated on two plant species, tomato and pepper, with or without nematode inoculation. Model calibration is a challenge, as it relies on heterogeneous and fairly scarce data. Indeed, plant experiments focusing on roots are necessarily destructive, hence the scarcity of data and the need to incorporate data from different experimental sources. The model was then used to analyse the complex interplay between plant physiological traits, phenology and nematode biology that affects system dynamics. Eventually, the model will help to identify the plant traits that characterize susceptible and tolerant plants, opening new perspectives for varietal selection.

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Age-structured Malaria Transmission Model

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Malaria is one of the vectorial diseases the most widespread in the world. Mainly located in tropical and subtropical regions, it causes hundreds of thousands of deaths every year. In this presentation, I will consider an epidemiological model [1] describing the malaria transmission between mosquitoes (female anopheles) and humans by considering different continuous structuring variables: chronological and infection ages and time since recovery. For this model, we first use integrated semigroups theory to ensure the existence and uniqueness of a nonnegative solution which is a bit delicate due to the singularity at zero of the force of infection. We will then focus of the derivation of the R_0 and the time-asymptotics behavior of the solution with a bifurcation study. Finally, we will discuss about existing data for the parameters of the model.

References

[1] Q. Richard, M. Choisy, T. Lefèvre, R. Djidjou-Demasse, *Human-vector malaria transmission model structured by age, time since infection and waning immunity*, Nonlinear Analysis: Real World Applications, 2022.

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Numerical Challenges for the Understanding of Snake-and-ladder Bifurcations in Nonlocal Hyperbolic Systems for Ecological Aggregations

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We consider a one-dimensional nonlocal hyperbolic model to understand group formation with application to self-organizing collectives of animals in homogeneous environments. Previous research has demonstrated that this model exhibits at least four complex spatial and spatiotemporal group patterns, as evidenced by numerical simulations and weakly nonlinear analysis. In this study, we focus on a type of complex bifurcation known as snake-and-ladder bifurcation which is characterized by the existence of localized solutions with different types of symmetries: even symmetry, odd symmetry, or non-symmetric solutions. To numerically construct the bifurcation solution branches, we employ different numerical schemes such as the upwind scheme, the MacCormack scheme, the Fractional-Step method, and the Quasi-Steady Wave-Propagation algorithm, combining them with high-resolution methods. We show several numerical issues in our study. Firstly, we observe the presence of two distinct types of numerical solutions that exhibit very small errors, which might initially suggest that we have reached a steady-state solution, but this is not the case. This also implies an extremely slow convergence. Secondly, in some cases, none of the investigated numerical schemes converge, posing a challenge to the numerical analysis. Lastly, we have discovered that the choice of numerical schemes, as well as their corresponding parameters such as time-space step and initial conditions, exert a significant influence on the type and symmetry of bifurcating solutions. As a result, the resulting bifurcation diagrams may vary when different numerical schemes and/or corresponding parameters are employed.

SPECIAL SESSIONS

SS1 - BIOMEDICINE MEETS NUMERICS: ADVANCED NUMERICAL METHODS FOR NEW CHALLENGES

Special Session

Organizers: Cristina Campi, Francesca Pitolli

Diagnosis and treatment techniques in biomedicine are becoming increasingly sophisticated. Advanced mathematical methods are essential for their development. This session aims to show how numerics has become an indispensable tool for the development of innovative methodologies for biomedical devices.

The participation to this session is open to all interested colleagues.

21st IMACS World Congress *University of Rome 'La Sapienza', Italy*

Session
Biomedicine Meets Numerics: Advanced Numerical Methods for New Challenges

Mathematical Methods in Medicine

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One of the new trends arising in oncological medical imaging is radiomics, a set of tools for the extraction of quantitative information from imaging data. The rationale beneath radiomics relies on the assumption that the quantitative information about morphological and functional descriptors that are computed form images in the early stage of the diagnostic process could be correlated with tumor-related genomic information. Yet, recently some papers [2, 1] critically discuss the reliability of radiomics as a systematic effective surrogate of genomics-based stratification and point out several pitfalls in this modern interpretation of quantitative radiology. In fact, radiomics descriptors are computed from a lesion that is extracted thanks to a segmentation algorithm, making the quantitative information dependent of the segmentation. The objective is to determine to what extent the accuracy of the segmentation approach impacts the accuracy of the radiomics features extracted from the segmented tumor district. From a mathematical view-point, there are very few studies about the reliability of the feature extraction procedure. In this talk we present measures for the quantitative assessment of the feature computation reliability with respect to the segmentation accuracy.

References

[1] J. E. Park et al., *A systematic review reporting quality of radiomics research in neuro-oncology: toward clinical utility and quality improvement using high-dimensional imaging features*, BMC Cancer 20 (2020), no. 1, 29.

[2] S. Rizzo et al., *Radiomics: the facts and the challenges of image analysis*, Eur. Radiol. Exp. 2 (2018), no. 1, 36.

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Session
Biomedicine Meets Numerics: Advanced Numerical Methods for New Challenges

A New TPS for FLASH VHEE Beams: the Implementation of Quantum Based Algorithms

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Over the past decades, technological advances have improved the efficacy of radiation therapy (RT) cancer treatments. Nevertheless, the RT potential is still far from being completely exploited. The techniques allowing for the best sparing of the normal tissue surrounding the target volume and the increase in the efficacy of the tumour killing are under continous research and development. The specific interactions of charged particles with matter can be exploited to achieve a particle therapy treatment capable of sparing the healthy tissues, while keeping the same target volume coverage. Recently, the interest in Very High Energy Electron (VHEE) beams have been renewed as they have enough energy to reach deep seated tumors and can represent a valid alternative to other external beam radiotherapy techniques like radiotherapy with photons and particle therapy delivered using protons or heavier ions. However, the availability of VHEE and other charged particles in the clinic has been hampered by the size, complexity, and ultimately high cost of the beam production system. In this context, the recent developments in the field of electron acceleration and FLASH radiotherapy are representing a promising perspective.The so called FLASH effect [1] has been observed when the plans are delivered at very high dose rates (larger than 10 Gy/s, to be compared with the 0.01 Gy/s of the conventional irradiation), very high dose per pulse ($10^6 Gy/pulse$) and high doses per fraction ($10 \sim Gy$ instead of the conventional 2 Gy). In FLASH conditions, it is possible to irradiate the healthy tissues reducing the normal tissue complication probability, allowing for a widening of the therapeutic window. In this respect, VHEE represent a perfect opportunity as they can be delivered at FLASH intensities already with the current existing facilities, while protons and photons have to face greater technological challenges.VHEE treatment planning plays thus a crucial role to demonstrate the feasibility and the potential of this projectile and require efficient and effective algorithms for the optimisation task. This abstract presents an innovative approach that combines Simulated Annealing (SA) [2] and Quantum Simulated Annealing (QSA) [3] algorithms as minimization methods to enhance the quality and efficiency of VHEE treatment plans. Traditional optimization algorithms often struggle to find optimal solutions due to the complexity and nonlinearity of the problem. In recent years, metaheuristic algorithms, such as Simulated Annealing (SA) and Quantum Simulated Annealing (QSA), have shown a promising performance in addressing this challenge. The proposed algorithm begins by formulating the treatment planning problem as an optimization task, aiming to minimize the objective function, accounting for the clinical criteria such as target coverage, critical structure sparing, and dose uniformity. The SA component of the algorithm employs a cooling schedule to explore the solution space, allowing for occasional uphill moves to avoid becoming trapped in local optima. To further improve the optimization process, the algorithm incorporates the QSA method, which utilizes principles of quantum mechanics to enhance the search for global optima. Quantum parameters, such as quantum fluctuations and annealing schedules, are carefully selected to balance exploration and exploitation of the solution space. Preliminary results on a real case of prostate cancer are presented demonstrating the potential of SA and QSA minimization methods implementation. By exploiting the strengths of both methods, this algorithm has the ability to overcome local optima and explore the solution space more effectively, allowing to achieve treatment plans that are better at achieving the clinical goals.

References

[1] Ronga MG, Cavallone M, Patriarca A, Leite AM, Loap P, Favaudon V, et al., *Very300 high-energy electrons (vhees) and their potential application in radiation therapy*, Cancers 13 (2021).301 doi:10.3390/cancers13194942.

[2] Goffe, William L., *SIMANN: A Global Optimization Algorithm using Simulated Annealing*, Studies in Nonlinear Dynamics and Econometrics, vol. 1, no. 3, 1996. https://doi.org/10.2202/1558-3708.1020.

[3] Chakrabarti Bikas K., Leschke Hajo, Ray Purusattam, Shirai Tatsuhiko and Tanaka Shu, *Quantum annealing and computation: challenges and perspectives*, Phil. Trans. R. Soc. A.3812021041920210419 http://doi.org/10.1098/rsta.2021.0419.

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Session
Biomedicine Meets Numerics: Advanced Numerical Methods for New Challenges

An In-vivo Comparison of Electrophysiological Source Imaging Methods

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Electrical source imaging (ESI) aims at reconstructing the electrical brain activity from measurements of the electric field on the scalp. ESI is a key element in the analysis of EEG data, in both research and clinical settings.
Over the past three decades, several algorithms have been developed to solve the ill-posed EEG inverse problem. The different methods mainly differ from each other by the quality and quantity of a priori information they use in order to solve the EEG inverse problem

In this study [1], we validate and compare ten different ESI methods by exploiting a recently published EEG dataset [2] recorded at Niguarda Hospital in Milan, Italy, for which the ground truth is known.

The main aim of this study was to assess the accuracy of the best reconstruction achieved by each method and analyze the impact of regularization parameters on the localization performance.

References

[1] Pascarella et al., An *in–vivo* validation of ESI methods with focal sources, 2023

[2] Mikulan et al, Simultaneous human intracerebral stimulation and HD-EEG, ground-truth for source localization methods, 2020

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Session
Biomedicine Meets Numerics: Advanced Numerical Methods for New Challenges

Advanced Computer Vision Techniques for Drug Abuse Detection

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Lateral flow tests, used to rapidly detect various diseases, as HIV, or specific physiological conditions, as drug abuse, through blood, saliva, or urine samples, are becoming a powerful and cost-effective diagnostic tool. One major factor affecting the test result is the subjectivity of the operator's reading, which relies on both the interpretation of the results and the assessment of sample compliance. To overcome this issue, Computer Vision (CV) provides tools to mitigate the subjectivity of the results. Indeed, through sophisticated CV algorithms, it is possible to calibrate and normalize the result interpretation, taking into account individual variations [1] and environmental influences.
In this talk, we present an automated lateral flow test reader for drug abuse detection, enabling both operator-independent interpretation of results and objective validation of sample compliance through CV techniques. One of the main challenges addressed in this study is to tackle the issue of non-uniform lighting in the analysis scene, while at the same time dealing with the variability in the positioning of the regions of interest. We propose an innovative method for objectively detecting the presence or absence of illicit substances, establishing a threshold for positivity and assessing the suitability of the analyzed sample, regardless of the limitations and subjectivity associated with the operator. A combination of filtering, image enhancement, and segmentation techniques were employed to extract relevant information. Additionally, color balancing and clustering methods were used to investigate the colors of sample suitability indicators. The results demonstrate the effectiveness of the proposed method in improving objectivity in rapid lateral flow test results.

References

[1] K.J. Emery, M.A. Webster, *Individual differences and their implications for color perception*, Current Opinion in Behavioral Sciences, Pages 28-33, 2019.

SS2 - COMPUTER SIMULATIONS IN DIGITAL TWINS TECHNOLOGY

Special Session

Organizer: Bharat Soni

Digital twin technology is one of the fastest growing concepts of Industry and healthcare. In the simplest terms, a digital twin is a virtual replica of a real-world object/asset/product/device/process/service/system/environment that is run in a simulation environment to test its performance outcomes, issues and efficacy. Hence, the benefits of Digital Twins include: accelerated risk assessment and production time, predictive maintenance, real-time remote monitoring, better team collaboration and better financial decision-making. In healthcare Digital Twin technology is applied to art of body/mind and social health.

Digital twins are highly complex models that use computational simulations, artificial intelligence (AI), machine learning, CAD, imagery, Extended Reality (VR, AR and MR), large amount of digital and physical data and blockchain techniques along with all aspects of IoT (Internet of Things). Abstracts are invited in any of the key technology areas influencing the progress in Digital Twins development and applications. In particular, the areas associated with Computational Simulations methodologies and applications involved in Digital Twins technology, AI, XR and management of a very large-scale BIG Data are encourarged.

Session
Computer Simulations in Digital Twins Technology

Digital Twin Technology in Maritime: MAAP Initiatives

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Following the fourth industrial revolution, and with the recent advances in information and communication technologies, the **digital twinning concept** is attracting the attention of both maritime academia and the maritime industry worldwide. A **digital twin** is a digital representation of a physical object, asset or system: a ship, a car, a wind turbine, a power grid, a pipeline, or a piece of equipment such as a thruster or an engine. One of the key initiatives at the MAAP is to apply **Digital Twin technology** in the development of MASS (Maritime Autonomous Surface Ship), e-navigation, ship engine room management, training and validation of operational concepts associated with smart and autonomous ships. To this end, the progress realized in adapting and exploring **digital twin** (DT) technologies at MAAP will be presented. In particular, **Kognitwin technology system** (a **Digital Twin system**) developed by Konsberg Maritime along with other systems applicable to decision making to ensure cost-effective, safer and sustainable operations will be described. The focus will be placed on using digital twin technology in some of the grey areas: Optimizing Fleet with Virtual Transition of Ship Control System, Enhancing the Port and Terminal Operations, Awareness of Situation with Regards to Operational Parameters, End-To-End Supply Chain Optimization, Amplified Security Ensuring Safety and Better vessel design and operation.

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Session
Computer Simulations in Digital Twins Technology

Non-Destructive Testing of 3D-Printed Parts Using Elastic Registration of Meshes in the X-ray Projection Domain

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Metrology inspection of complex parts produced by advanced manufacturing techniques such as additive manufacturing is challenging because these parts often contain inaccessible internal surfaces. In industry, quality control processes for parts with inaccessible surfaces wish to leverage X-ray tomography, which offers a non-destructive method to analyze measurement data in internal surfaces. However, X-ray tomography is a slow process and acquisition devices are costly. To address these cost and speed issues, we propose, instead of reconstructing surfaces through tomography, to leverage the information available from the CAD model of the analyzed part to compare surface definitions to manufactured surfaces directly in the X-ray projection domain. We therefore propose to deform a reference CAD model and subsequently analyze the deviations induced by various manufacturing processes. To do this, we use a limited number of X-rays to distort the CAD model, in the projective domain, so that it adapts to the actual part. Depending on the geometry of the part, we can suggest specific acquisition angles to minimize the number of X-rays needed to achieve the required measurement accuracy. Manufacturers will thereby have access to a quick method of comparing nominal and actual parts, using as few X-rays as possible. The technology developed is applicable and useful to a very large number of manufacturing fields, and constitute a concrete instance of digital twin technology applied in the field of manufacturing.

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Session
Computer Simulations in Digital Twins Technology

AI-assisted Dental Restorations

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Across North America, dentists install more than 2.5 million dental crowns each year, which represents a market above $4 billion by 2025. Each of these crowns must be designed manually by a specialized technician, which generates high costs, significant delays and great variability in the quality of the prostheses. In an effort to reduce cost and improve quality, we are pursuing the development of an AI-assisted software framework to support dentists in their interventions. Current results allow the generation of dental crowns for single teeth from a 3D scan of a patient's mouth. Work is now under way, through the development of advanced artificial intelligence models, to allow the treatment of more complex cases including the design of dental implants and bridges. Automatic methods are also being developed for designing dental preparations to provide references to dentists during their clinical interventions. This software framework provides computer tools capable of quickly and automatically generating high quality tooth restorations. These IT tools are being integrated into an automatic crown design application, which will be deployed to dentists directly in the clinic. This application will shorten the preparation times of prostheses for patients, reduce the costs of interventions and increase the quality and uniformity of the crowns produced. This software framework constitutes a concrete instance of digital twin technology applied in the field of health care.

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Session
Computer Simulations in Digital Twins Technology

Digital Twins Technology in Civil Engineering: Corrosion-Damage Detection on Concrete Structures

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Technological advancements are rapidly evolving and being implemented across various fields, including the construction industry. One such technological innovation is the digital twin, which creates a virtual replica of a physical object, process, or system to simulate real-world behavior. This study explores how digital twin technology can assist civil engineers in monitoring the condition of concrete infrastructure in real-time, focusing on detecting corrosion damage in common infrastructure such as columns, bridges, houses, and other concrete elements. The research utilizes a state-of-the-art framework that can accurately discretize damaged concrete elements, enabling earlier identification and prediction of potential failures and facilitating maintenance and replacement activities. The outcomes of this research demonstrate that real-time detection of corrosion damage through digital twin technology is highly accurate, outperforming traditional inspection methods. By leveraging this technology, civil engineers can detect and prevent more significant failures with greater precision, resulting in improved infrastructure maintenance and saving time and economic costs.

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Session
Computer Simulations in Digital Twins Technology

Development of Wind Tunnel Digital Twin Using Data Assimilation

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The "wind tunnel digital twin" is a technology that reproduces the airflow conditions of wind tunnel tests in numerical simulations based on Data Assimilation (DA), and is expected to be widely used in industries that require faithful evaluation of turbulent phenomena with high Reynolds numbers, such as aircraft development. Wind tunnel testing and numerical simulation have been major tools in recent aircraft development. The former has the advantage of high accuracy in reproducing turbulence, but has the disadvantages of high experimental cost and limitations on the location and amount of data that can be obtained. The latter is superior to wind tunnel testing in terms of installation cost and the amount of data that can be obtained, but has the problem of poor flow reproducibility due to the need to model turbulent phenomena. The wind tunnel digital twin will enable numerical simulations that faithfully represent the airflow of wind tunnel experiments, and will allow highly accurate fluid data to be acquired without being limited by the location or amount of data. This study demonstrates the effectiveness of the wind tunnel digital twin by using DA of Particle Image Velocimetry (PIV) measurements of the wake velocity field obtained from a wind tunnel test of a circular cylinder in which complex turbulent phenomena are observed, to bring the results of Detached Eddy Simulation (DES), which is suitable for reproducing unsteady turbulent flow, closer to the airflow of the wind tunnel tests. Although Large Eddy Simulation (LES) is available as an excellent unsteady simulation of turbulent flow, it has the disadvantage that the computational cost of high Reynolds number flows is too high. Therefore, DES, a low computational cost method that combines the Reynolds-Averaged Navier-Stokes (RANS) equations and LES was used. The approach of using two-dimensional PIV data to capture the unsteady structure of turbulence and then improving the accuracy of DES calculations by DA using the PIV data is unique to this study.

Session
Computer Simulations in Digital Twins Technology

Digital Twins Technology: Current Status and Future Directions

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Digital Twins technology is one of the fastest growing concepts of Industry and healthcare. In the simplest terms, a digital twin is a virtual replica of a real-world object/asset/product/device/process/service/system/environment that is run in a simulation environment to test its performance outcomes, issues and efficacy. Hence, the benefits of Digital Twins include: accelerated risk assessment and production time, predictive maintenance, real-time remote monitoring, better team collaboration and better financial decision-making. In healthcare Digital Twins technology is applied to science, practice and art of body-mind and social health.

Growth in IoT and cloud and the goal to cut down costs and reduce time for product development are the key factors driving growth in the digital twin market. The digital twin market is estimated to grow from $3.8 billion in 2019 to $35.8 billion by 2025, at a CAGR (Computed Average Growth Rate) of 37.8%. Digital Twins technology, combined with the latest machine learning and artificial intelligence tools, is helping companies across many industries to reduce operational costs, increase productivity, improve performance, and change the way predictive maintenance is done. For product manufacturers in particular, Digital Twins technology is crucial to achieving more efficient production lines and faster time-to-market.

Digital Twins are highly complex models that use artificial intelligence (AI), machine learning, CAD, imagery and Lidar, Extended Reality - XR (VR, AR and MR), large amount of digital and physical data, blockchain techniques, computational simulations along with all aspects of IoT (Internet of Things). The current status and future directions with a focus on healthcare applications will be described. In particular, innovations in XR towards the development of Digital Twins of human body, high fidelity computational simulations, big data and AI will be presented with applications.

SS3 - DELAY DIFFERENTIAL EQUATIONS AND APPLICATIONS

Special Session

Organizers: Eva Kaslik, Mihaela Neamţu

This session includes presentations concerning the applications of delay differential equations in areas ranging from biology, epidemiology and neurosciences, to population dynamics and economy. Interdisciplinary collaborations are welcome, as are recent advances in both discrete and continuous techniques, with special emphasis on mathematical models involving distributed time delays. This special session offers a dynamic platform for discussions, fostering collaboration and exchange of ideas among mathematicians, physicists, biologists, and engineers, among others.

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Session
Delay Differential Equiations and Applications

Dynamics Analysis of a Socioecological System

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The study proposes a dynamic analysis regarding interactions between the resources provided by the forest, the wildlife present inside or in the proximity of that environment and visitors revolving around the before mentioned socioecological framework. The mathematical model is described by a nonlinear system with three differential equations. The distributed time delay is introduced to illustrate the entire past impact of tourists on forest resources and wildlife. The basic assumption is that the wildlife species which inhabit the area are relying entirely on forest resources to meet their needs for food, shelter, and to attract tourists. Also, there is a positive correlation between ecotourism activities and the presence of forest resources and wildlife. The equilibrium points are determined, and they are subjected to a stability and bifurcation analysis, with particular emphasis on the positive equilibrium. The study employs a Hopf bifurcation analysis in the neighborhood of the equilibrium points by considering general delay kernels and choosing the average time-delay as the bifurcation parameter. The critical values of the average time-delay that lead to oscillatory behavior are determined. Numerical simulations are carried out to show the system's qualitative behavior in the vicinity of the equilibria.

References

[1] J. G. Villavicencio-Pulido1, V. Vázquez-Hipólito G. J. García-Cruz, Catastrophic or sustainable scenarios might occur when the carrying capacities of a tourism-based socioecological system vary, Natural Resource Modeling, (2022)

[2] E. Kaslik, M. Neamtu, Dynamics of a tourism sustainability model with distributed delay, Chaos, Solitons and Fractals 133, (2020)

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Session
Delay Differential Equiations and Applications

A Time-Delayed System of Identical Theta Neurons

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We consider an infinite network of identical theta neurons, all-to-all coupled by instantaneous synapses, modeled by a system of delay differential equations. We determine the number of equilibria with respect to κ and η, the characteristic parameters of the system and discuss the stability properties of each equilibrium and the possible bifurcations that may take place in the delayed system. Let us consider a network of N identical theta neurons, all-to-all coupled via a synaptic current I, which acts by injecting current into the neurons. We define the state of neuron j at time t as $\theta_j(t) \in [0, 2\pi]$. The dynamics of the network is given by the following system of N autonomous differential equations with distributed delay:

$$\dot{\theta}_j(t) = 1 - \cos\theta_j(t) + [1 + \cos\theta_j(t)]\,[\eta + \kappa(l * I)(t)]\,, \quad j \in \{1, 2, ..., N\} \tag{20}$$

where the synaptic current which acts on every neuron j of the network is

$$I(t) = \frac{1}{N}\sum_{n=1}^{N} [1 - \cos(\theta_n(t)]^2\,. \tag{21}$$

We note that the j-th represents the pulse of current emitted by j-th neuron as it fires.

The distributed time delay is introduced by the convolution $h*I$ defined as follows:

$$(l * I)(t) = \int_0^\infty l(s)I(t-s)ds,$$

where $l(s)$ is a probability density function.

Moreover, in the system defined, the constant parameter κ represents the overall coupling strength for the whole network, while η is the input current to each individual neuron, when uncoupled from the network.

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Session
Nonlinear Dynamics for Economics, Finance and Social Science

A Mixed Oligopoly Model with Time Delays

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The paper examines the interactions between a public firm and n private firms in the market using a discrete-time Cournot game framework with time delay. The objective of this study is to build upon previous research by examining how the stability of market equilibrium is affected by the presence of private firms and information delays. The investigation is motivated by the existence of mixed competition and the occurrence of multiple delays in the decision-making process. In this model, the production decisions of the public firm are influenced by the past output levels of the private firms. The production decisions of the private firms are influenced by both the past production levels of the public firm and the previous production levels of the other private firms. The nonlinear system under consideration has two equilibrium points: a positive equilibrium and a boundary equilibrium. Through stability analysis, it has been determined that the boundary equilibrium point functions as a saddle point. In the absence of delay, the stability region for the positive equilibrium point has been determined. Subsequently, by considering various specific cases of delays, the conditions under which the positive equilibrium becomes asymptotically stable have been identified. The primary outcome of this study is the determination of the stability of the Nash equilibrium concerning various factors.

We have also explored the flip and Neimark-Sacker bifurcations within the system. Numerical simulations have demonstrated that large time delays can result in complex dynamics and chaotic behavior.

Session
Nonlinear Dynamics for Economics, Finance and Social Science

Dynamics of a Pituitary-Adrenal Model with Distributed Time Delays

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The HPA axis, which serves as our primary stress response system, is regulated by various hormones, including corticotropin-releasing hormone (CRH), adrenocorticotropic hormone (ACTH), and cortisol (CORT) ([1]). This study aims to construct a two-dimensional model of the pituitary-adrenal axis, focusing on distributed time delays associated solely with ACTH and CORT. The model is based on findings from previous research ([2], which demonstrated that ultradian rhythms are generated autonomously, without reliance on CRH secretion.

We demonstrate the existence of a unique equilibrium point and analyze its local stability properties. By considering various types of delay kernels, we investigate the occurrence of Hopf bifurcations. A key finding of this research is the crucial role played by the choice of delay kernels in observing diverse dynamic phenomena. Additionally, we provide numerical simulations to validate the theoretical findings.

References

[1] E. Kaslik, M. Neamţu, *Stability and Hopf bifurcation analysis for the hypothalamic-pituitary-adrenal axis model with memory*, Mathematical Medicine and Biology: A Journal of the IMA, 35(1): 49–78, 2018.

[2] H. Malek, M. M. Ebadzadeh , R. Safabakhsh, A. Razavi, *Mathematical analysis of the role of pituitary- adrenal interactions in ultradian rhythms of the HPA axis.*, Computers in Biology and Medicine 135 : 104580, 2021.

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Session
Delay Differential Equations and Applications

Coupled Wilson-Cowan Systems with Distributed Delays

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The classical Wilson-Cowan model examines the interactions between excitatory and inhibitory meanfield dynamics in populations of neurons. It incorporates a weak Gamma distribution of time delays for input processing, which is derived through a time-coarse graining technique that averages the overall population response. Past investigations into the stability of the Wilson-Cowan model concentrated on simpler scenarios where delays were absent, constant, or followed a specific pattern. However, these simplifications can profoundly impact the model's behavior. Hence, our emphasis is on comprehending the system's behavior prior to time-coarse graining and across a broader spectrum of delay distributions.

In this paper, we consider a 4-dimensional model of two coupled Wilson-Cowan-type equations, with distributed time delays. We attempt to study the oscillation mechanism and frequency characteristics in the proposed model (EXN-INN-STN-GPe). For these generalized delay equations, we perform stability and bifurcation analyses with respect to parameters that capture both the coupling profile, and the time delay. The investigation is done through the examination of the system's associated characteristic equation.

Our findings demonstrate notable distinctions in stability regions and bifurcations across various delay distributions. Specifically, we observed that weak Gamma distributions encourage stable firing rates, whereas Dirac distributions tend to facilitate intricate and non-periodic patterns. These results suggest the intriguing prospect of employing different delay distributions as substrates for distinct functional behaviors, underscoring the significance of selecting an appropriate delay kernel in the mathematical model.

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Session
Delay Differential Equations and Applications

Stability and Hopf Bifurcation Analysis of an Unemployment Model with Distributed Time Delays

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This paper aims to construct and study a labor market model that incorporates both unemployment and underemployment. Underemployment refers to a situation where employees work fewer hours than their preferred level. The study takes into account the distributed time delays and its impact on policy responses. The research examines various aspects, including job separation, matching, transitions in and out of underemployment, and the potential for migration to an open economy with delayed policy intervention. The stability analysis focuses on the equilibrium of the corresponding dynamical system, with both Dirac and weak kernels. The theoretical findings are substantiated by numerical simulations.

References

[1] E. Kaslik, M. Neamtu, L.F. Vesa, Global stability analysis of an unemployment model with distributed delay, Mathematics and Computers in Simulation, in press, (2021)

[2] Misra, A.K. and Singh, A.K., A delay mathematical model for the control of unemployment. Differential Equations and Dynamical Systems, 21(3), 291-307 (2013)

[3] L. Harding, M. Neamtu, A dynamic model of unemployment with migration and delayed policy intervention, 51(3), 427-462 (2018)

SS4 - GRAPHICAL MODELS FOR LIFE SCIENCE

Special Session

Organizers: Claudia Angelini, Daniela De Canditiis, Italia De Feis

Graphical models are an elegant framework for describing complex systems of random variables. The nodes represent variables, while the edges represent relationships among variables, such as conditional independence. Bayesian networks are direct acyclic graphs, while Markov networks are undirect graphs, both have undergone enormous development in the last decades. Graphical models are helpful for the statistical analysis of data in various domains. Recently, they are becoming strategic for life science, allowing us to infer relations among variables such as genes/proteins/diseases/. However, their use in life science opens novel challenges due to the amount and heterogeneity of the data. This Special Session is open to theoretical and methodological contributions and innovative applications in life science.

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Session
Graphical Models for Life Science

Valid and Exact Two-sample Permutation Tests for Network Data

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We propose a general three-step procedure which entails the selection of: i) a model specification, ii) a network representation and iii) a network statistic of interest. Then, we introduce a novel class of two-sample Monte Carlo permutation tests for network data, suitable for any configuration chosen during the three steps. This general testing framework has the relevant feature, under weak assumptions, of being asymptotically valid and at the same time retaining the exact rejection probability α, in finite samples, when the underlying distributions of the two samples are identical. To test our novel procedure, we collected a random sample of 31 pregnant women from the study of *Della Rosa et al.* [1] who underwent resting-state functional magnetic resonance (rsf-MRI). The 31 participants were characterized by low risk (LR), $n = 19$ subjects, and high risk (HR), $m = 12$ subjects, for preterm birth (PTB), i.e. any birth occurring before the 37th week of gestation, based upon a multidimensional assessment and characterization of maternal risk profiles. The results of our permutation test, clearly show the presence of a different fetal brain functional connectivity in HR of PTB pregnancies compared to LR pregnancies. Thus we provide evidence that altered neurodevelopment, with differential fetal brain connectivity, is not a mere consequence of PTB, instead it can even anticipate birth.

References

[1] P. A. Della Rosa, C. Miglioli, M. Caglioni, F. Tiberio, K. H. H. Mosser, E. Vignotto, M. Canini, C. Baldoli, A. Falini, M. Candiani, P. Cavoretto (2021). *A hierarchical procedure to select intrauterine and extrauterine factors for methodological validation of preterm birth risk estimation.* BMC pregnancy and childbirth, 21(1), 306. https://doi.org/10.1186/s12884-021-03654-3

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Session
Graphical Models for Life Science

Structure Learning of Graphical Models for Count Data, with Applications to Single-cell RNA Sequencing

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The problem of estimating the structure of a graph from observed data is of growing interest in the context of high-throughput genomic data, and single-cell RNA sequencing in particular. These, however, are challenging applications, since the data consist of high-dimensional counts with high variance and over-abundance of zeros. Here, we present general frameworks for learning the structure of a graph from single-cell RNA-seq data. We demonstrate with simulations that our approaches are able to retrieve the structure of a graph in a variety of settings and we show the utility of the approach on real data.

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Session
Graphical Models for Life Science

Structure Learning of Coloured Gaussian Graphical Models for Paired Data

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Gaussian graphical models (GGMs) have become a popular tool in applications involving the joint learning of multiple networks, that is in the case where the observations come from two or more groups. The groups share the same variables and the interest is for the identification of similarities and differences between the networks associated with groups. In this context, the literature has mostly focused on the case where the groups are independent so that every network is a distinct unit, disconnected from the other networks, and only more recently on the case where groups are not independent. We considered the case of paired data, where there are exactly two dependent groups. Paired data commonly arise in paired design studies, where each subject is measured under two different conditions, or time points, as well as in matched observational studies. We firstly identify a family of coloured GGMs specifically suited for the paired data problem, and then approach the problem of learning the model from data by implementing of a penalized likelihood method, that we call the *symmetric graphical lasso* (SGL). The latter comprises two penalty terms: a graphical lasso penalty to induce sparsity in the graph structure, and then a fused lasso penalty to encourage both within-group and across-group symmetries. We illustrate the method with an application to the learning of a brain network from fMRI data where the two groups are represented by the two brain hemispheres.

References

[1] Ranciati, S., A. Roverato and A. Luati (2021). Fused graphical lasso for brain networks with symmetries. *Journal of the Royal Statistical Society: Series C (Applied Statistics) 70*(5), 1299–1322.

[2] Roverato, A. and D.N. Nguyen (2023). Exploration of the search space of Gaussian graphical models for paired data. *arXiv preprint arXiv:2303.05561*.

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Session
Graphical Models for Life Science

Empowering Propensity Score Estimation Through a Bayesian Network Approach

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In real world data the evaluation of treatment effect is a difficult task since the simple comparison of outcomes for treated vs control subjects is prone to bias: receiving a treatment is not a "purely random" event, and there could be relevant differences between treated and control subjects. This motivates the need to account for confounding covariates. Propensity score (PS) is a popular tool to account for this source of bias. Its use requires a careful modelling of the dependence relationships of the treatment on the covariates. Here we estimate PS using Bayesian Networks (BNs) that prove to be an excellent (generally better) alternative to the conventional logistic regression. When the actual dependence network in the data has a complex structure, logistic model leads to poor estimation of the PS and can even worsen the bias. The proposed PS estimator is then applied to the construction of two estimators of the Average Treatment Effect (ATE); the first one is of Horvitz-Thompson (HT) type, and the second one is of Hajek (H) type. They are also used as test-statistics for the hypothesis of absence of treatment effect. The two estimators are shown to be asymptotically equivalent provided the model for PS is correctly specified (this is always true in case of BNs). In case of specification errors, the H-type estimator proves to be better than the HT-type estimator. The properties of the proposed estimators are also studied through an extensive simulation study.

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Session
Graphical Models for Life Science

Random Graphical Model of Microbiome Interactions in Related Environments

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The microbiome constitutes a complex microbial ecology of interacting components that regulates important pathways in the host. Measurements of microbial abundances are key to learning the intricate network of interactions amongst microbes. Microbial communities at various body sites tend to share some overall common structure, while also showing diversity related to the needs of the local environment. We propose a computational approach for the joint inference of microbiota systems from metagenomic data for a number of body sites. The random graphical model (RGM) allows for heterogeneity across the different environments while quantifying their relatedness at the structural level. In addition, the model allows for the inclusion of external covariates at both the microbial and interaction levels, further adapting to the richness and complexity of microbiome data. Our results show how:the RGM approach is able to capture varying levels of structural similarity across the different body sites and how this is supported by their taxonomical classification; the Bayesian implementation of the RGM fully quantifies parameter uncertainty; the microbiome network posteriors show not only a stable core, but also interesting individual differences between the various body sites, as well as interpretable relationships between various classes of microbes.

SS5 - MATHEMATICAL AND COMPUTATIONAL METHODS FOR MIGRATION, AGGREGATION AND INTERACTION OF CELL POPULATIONS

Special Session

Organizers: Gabriella Bretti, Marta Menci

In recent years an increasing interest is registered in the field of modelling complex biological systems and developing techniques to combine experimental data and mathematical models, in order to develop in silico models that are able to reproduce and predict experimental outcomes. Indeed, the success of informed models is mainly due to the consistent improvements in computational abilities and in imaging techniques that allow a wider access to high spatial and temporal resolution data. In this framework, mathematical models and simulations describing the dynamics of cell populations in different applications (such as wound healing, organs-on-chip, tumor growth) with different approaches are presented.

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Session
Mathematical and Computational Methods for Migration, Aggregation and Interaction of Cell Populations

Dynamics of Circulating Tumor Cells in Blood Vessels: Mathematical Modeling and Data Assimilation

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Metastatic dissemination is a phenomenon that accounts for about 90% of deaths in cancer patients. A crucial step is when tumor cells from the primary tumor enter in the blood circulation and disseminate throught out the body, acquiring the name of circulating tumor cells (CTCs). Indeed, a small fraction of CTCs can survive and extravasate from a blood vessel but essential in colonizing a new organ, and then generating secondary colonies or metastasis. Before extravasation, we can observe a decrease in CTCs velocity and the arrest on the vessel wall due to the presence of two glycoproteins that create the adhesion links. Working in collaborations with a team of biologists of Goetz Lab for Tumor Biomechanics (Strasbourg), we aim to capture CTCs behaviour and the factors that mainly influence adhesion on the vessel wall.

The project focuses on *in vitro* experiments, where tumor cells are injected in a microfluidic channel (simulating a blood vessel) with controlled fluid velocity. Tracking CTCs in experimental videos, we can extract data such as CTCs trajectories and velocities. Cells and fluid velocity profiles can be reconstructed from these data throught a parameters estimation technique. The idea is to build a proper mathematical model consisting in an ODE-SDE system that well describes CTCs dynamics and, in particular, the links between adhesion forces and hemodynamics ones.

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Session
Mathematical and Computational Methods for Migration, Aggregation and Interaction of Cell Populations

Kinetic Models for Cell Migration in the Microenvironment: from the Microscopic to the Macroscopic Scale

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In this talk, I will illustrate a class of non-local kinetic models for cell migration in response to the external environment. In particular, we shall consider cell migration on the extra-cellular matrix (ECM) and two phenomena named contact guidance and steric hindrance depending on a single external cue (the ECM) that affects in a twofold way the polarization and speed of motion of the cells. We start from a microscopic description of the stochastic processes underlying the cell re-orientation mechanism related to the change of cell speed and direction. Then, we formally derive the corresponding kinetic model that implements exactly the prescribed microscopic dynamics and, from it, it is possible to deduce the macroscopic limit in the appropriate regime. Moreover, we test our model in several scenarios. In particular, we numerically investigate the minimal microscopic mechanisms that are necessary to reproduce cell dynamics by comparing the outcomes of our model with some experimental results related to breast cancer cell migration. This allows us to validate the proposed modeling approach and, also, to highlight its capability of predicting the qualitative cell behaviors in diverse heterogeneous microenvironments.

References

[1] Conte, M., & Loy, N. (2022). Multi-Cue Kinetic Model with Non-Local Sensing for Cell Migration on a Fiber Network with Chemotaxis. *Bulletin of Mathematical Biology*, **84(3)**. 1–46.

[2] Conte, M., & Loy, N. (2023). A non-local kinetic model for cell migration on the extracellular matrix by contact guidance and steric hindrance. *SIAP*, Accepted.

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Session
Mathematical and Computational Methods for Migration, Aggregation and Interaction of Cell Populations

GPU parallel numerical simulations of the Gatenby-Gawlinski model with with anisotropic, heterogeneous acid diffusion

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In this work we introduce a variant of the Gatenby-Gawlinski [1] model for acid-mediated tumor invasion, accounting for anisotropic and heterogeneous diffusion of the lactic acid across the surrounding healthy tissues. Numerical simulations are performed for two-dimensional data by employing finite volume schemes on staggered cartesian grids, and parallel implementation through the modern CUDA GPUs technology is considered [2],[3]. The effectiveness of such approach is proven by reproducing biologically relevant results like the formation of propagating fronts and the emergence of an interstitial gap between normal and cancerous cells, which is driven by the pH lowering strategy and depends significantly on the diffusion rates. By means of a performance analysis of the serial and parallel execution protocols, we infer that exploiting highly parallel GPU-based computing devices allows to rehabilitate finite volume schemes on regularly-shaped meshes, together with explicit time discretization, for complex applications to interface diffusion problems of invasive processes.

References

[1] Gatenby R.A., Gawlinski E.T., *A reaction-diffusion model of cancer invasion.*, Cancer Res. 56(24), 5745–5753 (1996)

[2] Kirk D.B., Hwu W.W., *Programming massively parallel processors: a hands-on approach. Third edition*, Morgan Kaufmann Publishers Inc., San Francisco (2016).

[3] Pera D., Malaga C., Simeoni C., Plaza R.G. , *On the efficient numerical simulation of heterogeneous anisotropic diffusion models for tumor invasion using GPUs.*, Rend. Mat. Appl. (7) 40(3-4), 233–255 (2019).

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Session
Mathematical and Computational Methods for Migration, Aggregation and Interaction of Cell Populations

Modelling Cell Migration: a Hybrid Approach for Cancer-on-chip Experiment

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In the last years a general class of hybrid models has been investigated, both from analytical and numerical perspective. The particular coupled structure has been introduced to model collective cell migrations under the influence of mechanical interactions and chemical stimuli. In this context, cells are modeled as discrete entities and their dynamics is given by ODEs, while the chemical signal influencing the motion is considered as a continuous signal which solves a diffusive equation. In this talk, we present recent advancements on a hybrid mathematical model inspired by Organs-on-chip technology and, in particular, in Cancer-on-chip experiment, where tumor cells are treated with chemotherapy drug and secrete chemical signals in the environment, thus stimulating immune response [1, 2]. The model improves previous works of the literature considering additional terms influencing the immune cells dynamics, together with a stochasticity component related to the motion of cancer cells. Multiple rigorous numerical schemes have been adapted or developed in order to simulate the coupled model. Several numerical simulations will be presented, in order to reproduce different scenarios, aiming at investigating the role of key parameters of the model on the overall dynamics.

This talk is based on joint works and ongoing collaborations in particular with Gabriella Bretti, Elio Campanile and Roberto Natalini.

References

[1] G. Bretti, A. De Ninno, R. Natalini, D. Peri, N. Roselli. *Estimation Algorithm for a Hybrid PDE–ODE Model Inspired by Immunocompetent Cancer-on-Chip Experiment*, Axioms 2021;10(4):243.

[2] G. Bretti, E. Campanile, M. Menci, R. Natalini. *A scenario-based study on hybrid PDE-ODE model for Cancer-on-chip experiment*, Problems in Mathematical Biophysics - a volume in memory of Alberto Gandolfi. SEMA SIMAI Springer Book Chapter.

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Session
Mathematical and Computational Methods for Migration, Aggregation and Interaction of Cell Populations

Large-scale Dynamics of Self-propelled Particles Moving through Obstacles: How Environment Affects Particle Swarms

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We investigate the collective motion of self-propelled agents in an environment filled with obstacles that are tethered to fixed positions via springs. The active particles are able to modify the environment by moving the obstacles through repulsion forces. This creates feedback interactions between the particles and the obstacles from which a breadth of patterns emerges (trails, band, clusters, honey-comb structures,...). We derive a macroscopic partial differential equations model from the agent-based dynamics describing the interactions between the self-propelled particles and the obstacles, under large tether stiffness. We perform an in-depth investigation of pattern formation of the discrete and continuum models in 2D: we provide phase-diagrams and determine the key mechanisms for bifurcations to happen using linear stability analysis. As a result, we discover that the agent-agent repulsion, the agent-obstacle repulsion and the obstacle's spring stiffness are the key forces in the appearance of patterns, while alignment forces between the particles play a secondary role. We present an innovative methodology to compare discrete and continuum models that we apply here to perform an in-depth analysis of the agreement between the discrete and continuum models.

SS6 - MATHEMATICS OF EMERGING AND RE-EMERGING HUMAN INFECTIOUS DISEASES OF MAJOR PUBLIC HEALTH IMPORTANCE

Special Session

Organizer: Jean Lubuma

Modeling of subsurface processes has a significant impact in many applications in agricultural, environmental and engineering context. These processes will be treated both in a physically based way, and in a data-driven fashion, always in the framework of porous media. For instance, novel numerical methods will be considered, as well as machine learning techniques based on real-life data, and control approaches for managing irrigation will be faced in a theoretical framework and with a simulation point of view. Subsurface processes are characterized by high non-linearities and even discontinuities, sometimes memory terms in differential equations, mainly in advection-diffusion PDEs. This session will bring together applied mathematicians and hydrologists studying applied flow and transport processes, to discuss novel modelling and numerical approaches for facing these difficulties. In particular, contributions will span among new modeling approaches for describing root water uptake with memory terms, mass conservative numerical methods for transport equations, control techniques in unsaturated flow equations, data-driven approaches for salt transport in agricultural soils, heterogeneous reactions in porous media, etc.

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Session
Mathematics of Emerging and Re-emerging Human Infectious Diseases of Major Public Health Importance

Mathematical Analysis of the Impact of the Face Mask on COVID-19

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We have modified and investigated the mathematical model introduced by [1]. The disease-free and endemic equilibrium stability analysis has been conducted. It has been proved that the DFE is globally asymptotically stable when the basic reproduction number $\mathcal{R}0 \leq 1$. The proposed model has a unique endemic equilibrium globally asymptotically stable whenever $\mathcal{R}0 > 1$. A numerical simulation illustrates the theoretical results.

References

[1] E. A. Iboi, O. Sharomi, C. N. Ngonghala, A. B. Gumel. Mathematical modeling and analysis of COVID-19 pandemic in Nigeria. *Mathematical Biosciences and Engineering*, 2020, 17, (6): 7192-7220.

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Session
Mathematics of Emerging and Re-emerging Human Infectious Diseases of Major Public Health Importance

Some Qualitatively Reliable Models for Epidemic Spread

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A model of a biological/physical system corresponds to the construction of an approximate mathematical representation of the system, incorporating certain important and essential features of the system, while ignoring everything else [1]. Thus, different classes of models are distinguished by which features are reproduced by the model. We consider some continuous and discrete mathematical models for the epidemic spread. The continuous models are typically some Cauchy problems for systems of ordinary differential equations, while the discrete models are obtained by their suitable time discretization.

A fundamental criterion for these models is that they include the most important qualitative properties of the original phenomenon. These properties are biologically motivated for the epidemic spread process. Therefore our first aim is to construct reliable continuous models. A further goal is to use such discretization procedures that result in a discrete model which preserve these qualitative properties.

In our talk for the discretization we use the combination of an ERK method with the nonstandard finite difference (NSFD) method [2]. We show that this combined method does not only preserve the consistency order and convergence of the base ERK method but also have many other good qualitative features. We demonstrate our theoretical results on different models.

References

[1] M.B. Allen, I. Herrera, and G.F. Pinder. *Numerical modeling science and engineering*, Wiley, New York, 1988

[2] R.E. Mickens. *Dynamic consistency: A fundamental principle for constructing nonstandard finite difference schemes for differential equations.* Journal of Difference Equations and Applications, 11 645–653, 2005

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Session
Mathematics of Emerging and Re-emerging Human Infectious Diseases of Major Public Health Importance

Age-structured Mathematical Models Based on Nonlinear ODEs to Study the Optimality of Vaccination Strategies for COVID-19 Pandemic

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In this research we present a variety of mathematical models that are useful to study different vaccination strategies. The models are based on relatively large nonlinear non-autonomous systems of differential equations. The proposed epidemiological models take into account various demographic factors and specific functions for the vaccination distribution. In order to investigate the optimal vaccination strategies we use the number of deaths as the metric to measure the efficacy of each of the strategies. The mathematical models include a large number of parameters and variables, which makes the problem of finding the optimal strategy a very complex one. The constructed mathematical models include different demographic factors such as age, sex, comorbidity status and social contacts of the population. We numerically solve the nonlinear systems in order to assess the optimality of a large number of strategies that differ on the vaccination priority of each demographic group. The results of this research give further insight about the relevance of the vaccination strategies that allow to reduce deaths due to the COVID disease. The problem of selecting the optimal vaccination strategy is remarkably complex due to the large number of aspects that need to be considered, including also high dimensionality and nonlinearities. The outcomes of this research show that the optimal strategy varies depending on the prevalent transmission rates of SARS-CoV-2. For low transmission regions the optimal strategy gives vaccination priority to demographic groups with high transmission rates and for high transmission regions, the vaccination priority is for groups with high fatality rates.

21st IMACS World Congress *University of Rome 'La Sapienza', Italy*

Minisymposium
Mathematics of Emerging and Re-emerging Human Infectious Diseases
of Major Public Health Importance

A Metapopulation Model for the 2014-2016 West Africa Ebola Virus Disease Outbreak, Part II: Optimal Control Strategies

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The 2014-2016 West Africa Ebola Virus Disease (EVD) is the largest and severest outbreak, with a total of 28,616 cases and 11,310 deaths reported. It arose in three different countries, namely Guinea, Liberia and Sierra Leone, in which migrations and travel of people by road and air were considerable.

We construct a metapopulation model to study the transmission dynamics as well as the control and management of the disease. In each patch, we consider an extended Susceptible-Exposed-Infective-Recovered ($SEIR$) type-model enriched by compartments D, P and Q that account for disease induced deceased, isolated and quarantined individuals, respectively.

In this second presentation of a series of two, we consider two optimal control problems. The first problem is defined through the exit-entry screening of travelers. The second problem is articulated around the combination of the exit screening and the vaccination interventions. The well-posedness of both optimal control problems is proved and implemented by Pontryagin's maximum principle.

For each optimal control problem, we construct a new Forward-Backward-Sweep-Method (FBSM) with clearly defined iterations, $k = 0, 1, \cdots$. The state variable system is approximated by a nonstandard forward Euler scheme, which is shown to be dynamically consistent with respect to the continuous model. The adjoint system is discretized by the classical backward Euler scheme. It is shown that the new FBSM is convergent. Numerical simulations that support the theory are provided.

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A Metapopulation Model for the 2014-2016 West Africa Ebola Virus Disease Outbreak, Part I: Exit Screening and Quarantine Measures

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The 2014-2016 West Africa Ebola Virus Disease (EVD) is the largest and severest outbreak, with a total of 28,616 cases and 11,310 deaths reported. It arose in three different countries, namely Guinea, Liberia and Sierra Leone, in which migrations and travel of people by road and air were considerable.

We construct a metapopulation model to study the transmission dynamics as well as the control and management of the disease. In each patch, we consider an extended Susceptible-Exposed-Infective-Recovered ($SEIR$) type-model enriched by compartments D, P and Q that account for disease induced deceased, isolated and quarantined individuals, respectively.

In this first presentation of a series of two, we analyse the impact of the exit screening of travelers, recommended by the World Health Organization in 2014. To this end, we suitably incorporate into the model well-defined parameters for the exit screening of travelers, the quarantine of positively screened travelers and the migration/travel between patches.

We compute the control reproduction number, $\mathcal{R}_c$, thanks to which the local asymptotic stability (LAS) and instability of the disease-free equilibrium (DFE) is established whenever $\mathcal{R}_c < 1$ and $\mathcal{R}_c > 1$, respectively. For global stability, we introduce an additional threshold number, $\mathcal{T}$, that is greater than $\mathcal{R}_c$. It is proved that the DFE is globally asymptotically stable (GAS) when $\mathcal{T} < 1$, while there exist patch boundary equilibrium points when $\mathcal{T} > 1$, and their LAS is discussed.

We construct a nonstandard finite difference scheme that is dynamically consistent with the properties of the continuous model. Numerical simulations obtained from real data are provided to support the theory.

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Mathematics of Emerging and Re-emerging Human Infectious Diseases
of Major Public Health Importance

SEIR Epidemic Mathematical Model in the Presence of Hoax

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In this paper we present a mathematical model for the transmission of a contagious disease. We explore the effect of disinformation such as rumour and hoax regarding the disease into the spread of the disease infection. This phenomea is not uncommon to occur, such as in the case of COVID-19 pandemic. There are so many misinformation or even disinformation regarding the nature of the disease and how people should behave toward the disease. In the beginning of COVID-19 pandemic some rumours and hoaxes about the disease are circulated. In many countries this led to mismanagement of the disease, in particular many people exhibited poor behaviour or poor disease awareness in responding to the disease. We propose a mathematical model in the form of differential equation to describe how a contagious disease spread in the presence of rumour and hoax. By modifying the known SEIR model, we divide the population into different categories depending on their health status, such as susceptibles, infected and immune individuals. Furthermore, we also divide the susceptibles into different categories according to the knowledge of the rumour and hoax, i.e. susceptibles that have not heard the rumour (ignorant), susceptibles that have heard the rumour and also spread the rumour (spreader), susceptible that have heard the rumour but do not spread the rumor anymore (stifler). A standard dynamical analysis is carried out to study the behaviour of the model. In this case we present the equilibria for the model and show their stabilities and their relationship to the basic reproduction number. A critical level of intervention in order to reduce the infection will also be presented.

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Mathematics of Emerging and Re-emerging Human Infectious Diseases
of Major Public Health Importance

Positivity Preserving Numerical Methods Applied to Epidemic Models

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In recent years the importance of mathematical modeling of propagation of illnesses was highlighted by the outbreak of the Covid-19 epidemic. In this talk we observe an SEIR model (describing the propagation of an illness in a population) with a general incidence rate. Although the qualitative properties of such models were widely studied before (see e.g. [1]), the proper choice for a numerical method which preserves the properties of the original, continuous system remains a crucial problem. In this talk we propose several different methods: strong stability preserving Runge-Kutta methods [3] along with lower and higher order non-standard methods [2, 4]. We give different conditions under which the numerical schemes behave as expected. Then, the theoretical results are demonstrated by some numerical experiments.

References

[1] A. Bernoussi. Global stability analysis of an SEIR epidemic model with relapse and general incidence rates. *Appl. Sci*, 21, 54–68, 2019.

[2] Q. A. Dang, M. T. Hoang. Positive and elementary stable explicit nonstandard Runge-Kutta methods for a class of autonomous dynamical systems. *International Journal of Computer Mathematics*, 97(10), 2036–2054, 2020. https://doi.org/10.1080/00207160.2019.1677895

[3] S. Gottlieb, D. I. Ketcheson, C-W. Shu. Strong stability preserving Runge- Kutta and multistep time discretizations. *World Scientific Publishing Co. Pte. Ltd., Hackensack, NJ*, 2011. https://doi.org/10.1142/7498.

[4] R. E. Mickens. Advances in the applications of nonstandard finite difference schemes. *World Scientific*, 2005.

SS7 - MODELING HUMAN PERCEPTION OF VISUAL INFORMATION

Special Session

Organizer: Giuliana Ramella

In everyday life, Machine Vision has made significant progress toward becoming more pervasive due to recent developments in artificial intelligence and computing capabilities. Despite the tangible and excellent results, the current Machine Vision techniques fall short of our expectations compared to the ease with which the Human Visual System (HVS) deals with complex scene analysis and abstraction. Thus, we are witnessing a growing interest in HVS-inspired approaches for developing more thoughtful and efficient visual information modeling and processing methods. The Mini-Symposium aims to bring together leading scientists to present their latest HVS-inspired practices and to establish new directions for future investigations and cooperation. We welcome contributions using tools including (but not restricted to): Applied Harmonic Analysis, Compression Methods, Geometric and Topological Techniques, Mathematical Morphology, Partial Differential Equations, Probabilistic and Statistical Methodologies, Interpolation Methods, Multiresolution Analysis, and Variational Methods for applications related to Signal and Image Processing, Pattern Recognition, and Visual Machine Learning

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Session
Modeling Human Perception of Visual Information

An Image Segmentation Approach for Space Syntax and Urban Mobility

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Space syntax is a set of techniques for analyzing spatial layouts and human activity patterns in buildings and urban areas, together with a set of theories linking space and society. As Space is described in terms of discrete spatial elements that relate to human behavior it is usually represented with graphs and analysed with graph theory techniques since relationships between spatial elements result from their configuration. These relationships can be objectively analysed using various centrality measures, included among which are integration and choice. In this contribution, we supplement these measures by weighting them according to the presence of buildings and greenery, using image segmentation.

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Session
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Hierarchical Segmentation of Cell Compartments in Electron Microscope Images

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Image segmentation is one of the most demanding problems in the computer vision area. In recent years, due to the development of neural network based methods (e.g., deep learning, convolutional neural networks), significant progress has been made in this area. However, the use of such methods for less commonly analysed types of images encounters many problems. This situation encourages attempts to develop dedicated segmentation algorithms based on more traditional methods of image processing and analysis. During the development of such algorithms, it is worth paying attention to how the human vision system (HVS) operates when analysing a new type of image. In this case, HVS demonstrates the ability to perform a quick rough analysis of unknown images.

In this study, we present a relatively simple segmentation algorithm partially inspired by HVS for the segmentation of images of a human colorectal carcinoma cell acquired using electron microscopy imaging. The purpose of segmentation is to separate image regions representing the background, cells and cell nuclei. This aim is realised hierarchically, i.e., in the first stage the cells are separated from the background and then for each cell's region, its cell nucleus region is separated. To achieve this, the developed algorithm used, among others, images with different degrees of detail and region-based segmentation methods. The algorithm has been tested with images of the HCT116 cell line and the obtained results show good consistency with the results provided by experts.

The purpose of further research will be to adapt the presented algorithm to segmentation of cell images for cell lines other than HCT116. It is also planned to develop this algorithm to segment elements of the cellular ultrastructure other than the cell nucleus. It is also worth noting that the presented algorithm can be used to speed up the image annotation process to prepare the data necessary for training a neural network.

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A Perception-guided CNN for Grape Bunch Detection

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Smart farming is becoming an active and interdisciplinary research field as it requires to solve interesting and challenging research issues to respond concretely to the demands of specific use-cases. One of the most delicate tasks is the automatic yield estimation, as for example in vineyards [1]. Computer vision methods that implement the rules of the human visual system can contribute to task accomplishment as they simulate what winemakers make manually [2]. An automatic artificial-intelligence method for grape bunch detection from RGB images is presented. It properly defines the input of a Convolutional Neural Network whose task is the segmentation of grape bunches [3]. The network input consists of pointwise visual contrast-based measurements that allow us to discriminate and detect grape bunches even in uncontrolled acquisition conditions and with limited computational load. The latter property makes the proposed method implementable on smart devices and appropriate for onsite and real-time applications.

References

[1] V. Bruni, D. Vitulano, Z. Wang, *Special issue on human vision and information theory*, Signal Image Video Processing, 2013.

[2] V. Bruni, G. Dominijanni, D. Vitulano, *A Machine-Learning Approach for Automatic Grape-Bunch Detection Based on Opponent Colors*, Sustainability, 2023.

[3] J. Gu, T. Liu, X. Wang, G. Wang, J. Cai, T. Chen, *Recent Advances in Convolutional Neural Networks*, Pattern Recognition, 2018.

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Session
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Contrast-based Image Enhancement for Source Camera Identification

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Source camera identification is a challenging problem in forensics applications. It consists of capturing the fingerprint that the acquisition device leaves in each acquired image. The fingerprint is mainly represented by a multiplicative noise source, namely the Photo Response Non Uniformity (PRNU) pattern noise, that uniquely identifies device acquisition sensor. Due to its nature, conventional approaches address the issue as a denoising problem where the residual image is the PRNU [1]. However, several problems arise, including the selection of the best denoiser that greatly influences the successive recognition step. Based on these considerations, a recognition method that directly works on the original image is investigated. It mainly takes advantage of the multiplicative nature of PRNU, which therefore leaves PRNU basically unchanged in the flat regions of the image [2, 3]. To emphasize this property, contrast enhancement is applied block-wise and enhanced image blocks are treated as independent images to classify using a Convolutional Neural Network. Preliminary results achieved on benchmark datasets will be presented along with an evaluation study concerning the influence of contrast enhancement.

References

[1] J. Lukas, J. Fridrich, M. Goljan, *Digital camera identification from sensor pattern noise*, IEEE Trans. on Information Forensics and Security, 2006

[2] V. Bruni, M. Tartaglione, D. Vitulano,*Coherence of PRNU weighted estimations for improved source camera identification*, Mult. Tools & Appl., 2022.

[3] M. Tiwari, B.Gupta, *Image features dependant correlation-weighting function for efficient PRNU source camera identification*, Forens. Sc. Int., 2018.

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Session
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Application of Fractional Derivatives in Image Quality Assessment Indices

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Objective image quality assessment involves the use of mathematical models to quantitatively describe image quality. FR-IQA (Full-Reference Image Quality Assessment) methods using reference images are also often used to evaluate image processing and computer vision algorithms. The quality index must take into account both local and global information and perform their integration. These indices often use gradient operators to express relevant visual information, e.g., edges. Fractional calculus has been applied in the last two decades in various fields such as signal processing, image processing, and pattern recognition. Fractional derivatives are a generalization of integer-order derivatives and can be computed using various operators such as the Riemann-Liouville, Caputo, and the Grünwald-Letnikov operators [1]. In this paper, we propose a modification of the FSIMc image quality index [2], by including fractional derivatives to extract and enhance edges. Using an appropriate operator, fractional derivatives are calculated for each pixel, gradient maps are built by calculating the magnitudes and directions of the fractional derivatives and used to calculate the index. A study of the usefulness of the fractional derivative in the FSIMc model was conducted by assessing Pearson, Spearman, and Kendall correlations with MOS scores for images from the TID2013 database. The results encourage the use of fractional calculus.

References

[1] D. Varga, Full-Reference Image Quality Assessment Based on Grünwald–Letnikov Derivative, Image Gradients, and Visual Saliency. Electronics, 2022, 11(4), 559.

[2] L. Zhang, L. Zhang, L. Mou, D. Zhang, FSIM: A Feature Similarity Index for Image Quality Assessment. IEEE Trans. Image Process. 2011, 20, 2378–2386.

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Session
Modeling Human Perception of Visual Information

Regular Shapes on Surfaces: Angles, Lengths, and How They Are Perceived

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The perception of angles, lengths, and aspect ratios characterizes the visual understanding of planar shapes [1]. Indeed, sensitivity to geometric shape regularity seems to be a distinctive characteristic of human perception [2].
We study the perception of shapes drawn on a curved surface embedded in 3D space. In this case, geodesic polygons provide a natural counterpart of Euclidean piecewise linear shapes. However, the relations between lengths and angles of such polygons involve the Gaussian curvature of the host surface, producing shapes that contrast our perception of regularity. For instance, it is generally impossible to obtain polygons with equal edge lengths *and* equal angles; or quadrilaterals with all right angles. Besides, depending on the curvature of the host space, equilaterar polygons may appear to be either "fatter" or"thinner" than their Euclidean counterpart.
We investigate polygons on surfaces of constant curvature, showing that they preserve some regularity, and we provide visual examples on general free-form surfaces with varying curvature. We show that the visual perception of geodesics as *straightest* lines is often mistaken. We propose the concept of *as-geodesic-as-possible* polygons, expressing it as an optimization problem: we trade-off the null geodesic curvature of the sides to have more leeway on the angles. We argue that such polygons are perceived as more regular and similar to their planar counterpart than the corresponding geodesic polygons.

References

[1] V. Izard, P. Pica, E.S. Spelke, 2022, Visual foundations of Euclidean geometry, *Cognitive Psychology*, 136, 101494.

[2] M. Sablé-Meyer, J. Fagot, S. Caparos, T. van Kerkoerle, M. Amalric, and S. Dehaene, 2021, Sensitivity to geometric shape regularity in humans and baboons: A putative signature of human singularity, *PNAS*, 118(16).

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Session
Modeling Human Perception of Visual Information

Advances in a Quantum Information-based Color Perception Theory

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Color perception has been a topic of interest for an astonishing number of scientists, philosophers, poets and painters. Scientifically speaking, from the publication of Newton's Opticks in 1704 to Schrödinger's 1920 axiomatic system, top-level physicists and mathematicians, as Young, Maxwell, Grassmann and von Helmholtz, contributed to clarify the nature of color.

The advent of the CIE (Commission International de l'Éclairage) and its color reproduction model based entirely on the photoreceptors sensitivities created a cultural hiatus with the initial ideas of the founding fathers of colorimetry.

This explains why Schrödinger's axiomatic system was completed only in 1974 by H.L. Resnikoff, who paved the way for a new era of colorimetry. His splendid work, however, remained ignored for more than 40 years.

In this lecture I will show how, by re-interpreting Resnikoff's work in the setting of quantum information, it is possible to explain a vast number of phenomenological facts about color perception and to predict new ones.

In particular, I will show how the algebraic formalism of density matrices permits to reconcile trichromacy with Hering's opponent theory in a natural way and to replace the circular and heuristic definitions of color attributes given by the CIE with a coherent and rigorous new vocabulary. [1] and [2] are the most recent references of this research program in collaboration with Michel Berthier.

References

[1] M. Berthier and E. Provenzi. Quantum measurement and colour perception: theory and applications. *Proceedings of the The Royal Society A*, 478(2258):2021050, 2022.

[2] M. Berthier, N. Prencipe and E. Provenzi. A Quantum Information-Based Refoundation of Color Perception Concepts. *SIAM Journal on Imaging Sciences*, 15(4):1944-1976, 2022.

SS8 - NEW TRENDS IN PHASE FIELD: THEORY AND APPLICATIONS

Special Session

Organizers: Mejdi Azaiez, Chuanju Xu

The phase field method is a powerful numerical method to solve moving boundary problems appearing in Materials Science and Engineering. Its application covers from solidification of pure materials to crystal Modeling. Phase field theories are parameterized by a set of physically motivated variables that have a continuous spatial variation between the equilibrium values of the phases which adjoin the interface.

Interfacial dynamics in complex fluids presents tremendous challenges to science. From a fluid mechanical viewpoint, the essential physics is the coupling between interfacial movement and the flow of the bulk fluids. Phase field (diffuse-interface) methods start from a multi-scale point of view and treat the interface as a microscopic transition zone of small but finite width. Then a set of governing equations can be derived that are thermodynamically consistent and mathematically well-posed.

This principle is very powerful and flexible. It has been applied successfully to describe complicated interfaces in various complex fluids. Well designed numerical methods with the diffuse-interface approach can be highly robust and accurate, as long as the interface is well resolved. Phase field methods are now widely used in many branches of science and engineering, such as the material science, biomedical science, biology, chemical engineering.

This mini-symposium will bring together numerical analysts and computational scientists working on phase field methods to present their recent advances in algorithm designs and applications of phase field methods. The main purposes of this mini-symposium are to review the current status, identify problems and future directions, and to promote phase field methods to a wider scientific and engineering community.

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Session
New Trends in Phase Field: Theory and Applications

Nonlocal Cahn-Hilliard type Model for Image Inpainting

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This talk proposes a Cahn-Hilliard type inpainting model equipped with a nonlocal diffusion operator. A rigorous analysis of the well-posedness of the stationary solution is established using Schauder's fixed point theory. We construct a numerical scheme based on the convexity splitting method with the nonlocal term treated implicitly and the fidelity term treated explicitly. We prove the consistency, stability and convergence of the scheme. To the best of our knowledge, this is the first study to present such an analysis and numerical scheme for this model, which provides valuable guidance for parameter selection. Numerical experiments validate the effectiveness of the proposed nonlocal model, which shows superior performance compared to both local and classical total variation models in preserving fine textures and recovering image edges.

References

[1] Bertozzi, Andrea L and Esedoglu, Selim and Gillette, Alan, *Inpainting of binary images using the Cahn–Hilliard equation*, IEEE Transactions on image processing, 2006.

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Session
New Trends in Phase Field: Theory and Applications

Monte Carlo fPINNs: Deep Learning Method for Forward and Inverse Problems Involving High Dimensional Fractional Partial Differential Equations

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In this talk, we will present a sampling-based machine learning approach, Monte Carlo fractional physics-informed neural networks (MC-fPINNs), for solving forward and inverse fractional partial differential equations (FPDEs). As a generalization of the physics-informed neural networks (PINNs), MC-fPINNs utilize a Monte Carlo approximation strategy to compute the fractional derivatives of the DNN outputs, and construct an unbiased estimation of the physical soft constraints in the loss function. Our sampling approach can yield lower overall computational cost compared to fPINNs, hence it can solve high dimensional FPDEs at reasonable cost. We validate the performance of MC-fPINNs via several examples and the results show that MC-fPINNs are flexible and quite effective in tackling high dimensional FPDEs.

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Session
New Trends in Phase Field: Theory and Applications

A Diffuse Domain Method for Solving PDEs in Complex Geometries

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We will present a diffuse domain approach for solving PDEs in complex, involving domain. The approach extends the original complex domain into a larger and regular domain, where the original PDEs are extended and solved. The original boundary conditions are absorbed as a source term into the reformulated equations. Several numerical examples including multiphase flows, the epitaxial growth of two-dimensional material with anisotropy are shown to illustrate the approach.

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Session
New Trends in Phase Field: Theory and Applications

A Unified Design of Nonuniform Energy Stable Schemes for Time Fractional Gradient Flows and Nonlinear Integro-differential Equations

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A unified discrete gradient structure of the second order nonuniform integral averaged approximations for Caputo fractional derivative and Riemann-Liouville fractional integral is established. The required constraint of the step-size ratio is weaker than that found in literatures. With the proposed discrete gradient structure, the energy stability of the variable-step Crank-Nicolson type numerical schemes is derived immediately, which is essential to the long-time simulations of the time fractional gradient flows and the nonlinear integro-differential models. The discrete energy dissipation laws fit seamlessly into their classical counterparts when the fractional indexes tend to 1. In particular, it provides a framework for the energy stability analysis of the variable-step numerical schemes based on the scalar auxiliary variable type approaches. The time fractional Cahn-Hilliard model and the time fractional sine-Gordon model are taken as two examples to elucidate the theoretical results at great length. Extensive numerical experiments using the adaptive time-stepping strategy are provided to verify the theoretical results in the time multi-scale simulations.

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Session
New Trends in Phase Field: Theory and Applications

On Operator Splitting Methods for Phase-field Equations

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We consider a class of second-order Strang splitting methods for Allen-Cahn equations with polynomial or logarithmic nonlinearities. For the polynomial case both the linear and the nonlinear propagators are computed explicitly. We show that this type of Strang splitting scheme is unconditionally stable regardless of the time step. Moreover we establish strict energy dissipation for a judiciously modified energy which coincides with the classical energy up to $\mathcal{O}(\tau)$ where τ is the time step. For the logarithmic potential case, since the continuous-time nonlinear propagator no longer enjoys explicit analytic treatments, we employ a second order in time two-stage implicit Runge–Kutta (RK) nonlinear propagator together with an efficient Newton iterative solver. We prove a maximum principle which ensures phase separation and establish energy dissipation law under mild restrictions on the time step. These appear to be the first rigorous results on the energy dissipation of Strang-type splitting methods for Allen-Cahn equations.

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Session
New Trends in Phase Field: Theory and Applications

Gradient Flow Models: Modeling and Numerical Methods

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In this talk I will discuss a variety of gradient flow models for multi-phase problems, derived from an energy variational formulation. The models can be used to describe fracture of composite materials, PCM, the interfacial dynamics of immiscible and incompressible two-phase fluids, anisotropic phase-field dendritic crystal growth model, abnormal diffusion interfaces, etc. The talk starts with a review of the models and numerical methods for these models. Then a new class of efficient time-stepping schemes will be discussed.

Key words: Gradient flows; phase field modeling; numerical methods

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Session
New Trends in Phase Field: Theory and Applications

Numerical Modelling and Optimization for Thermal Energy Storage

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Composite phase change materials (CPCMs) refer to materials formed by combining phase change materials with highly thermally conductive materials such as graphite and copper foam, aiming to enhance heat/cool storage efficiency. We develop a toolbox based on the finite element software `FreeFEM`, enable to simulate the solidification and melting phenomena of CPCMs from a microscopic perspective. Our model is based on the phase field method, with a penalty technique to describe complex porous structures. Our model only requires solving one temperature variable while satisfying the temperature jump at material interfaces due to thermal resistance. We design a numerical scheme which decouples the phase field and temperature. In space disretization, a hybrid finite element method is applied to meet the exsitence of temperature jump. In implementation, we employ the domain decomposition library `ffddm` for parallelization and `Mmg` module for mesh refinement to improve the efficency. Simulations for melting/freezing processes on different porous structure CPCMs are presented to validate our model.

References

[1] F. Hecht. New development in freefem++. J. Numer. Math., 20(3-4):251–265, 2012.

[2] P.-H. Tournier, P. Jolivet, and F. Nataf. FFDDM: Freefem domain decomposition method. https://doc.freefem.org/documentation/ffddm/index.html, 2019.

[3] G. Sadaka, A. Rakotondrandisa, P.-H. Tournier, F. Luddens, C. Lothode, and I. Danaila. Parallel finite-element codes for the simulation of two-dimensional and three-dimensional solid–liquid phase-change systems with natural convection. Comput. Phys. Commun., 257:107492, 2020.

SS9 - NONLINEAR DYNAMICS FOR ECONOMICS, FINANCE AND SOCIAL SCIENCES

Special Session

Organizer: Fabio Tramontana

This Session hosts theoretical works where models are formulated via differential or difference nonlinear equations. Also, piecewise-defined dynamic equations are welcome. These models must have an application to economic, financial or social problems. Here is a, non exhaustive, list of topics:

- Nonlinear dynamics
- Dynamic models for growth, endogenous oscillations, stability and bifurcations of social systems
- Dynamic models in discrete and continuous time for economics, finance, environment, behavioral economics
- Differential games
- Chaos control, chaos synchronization
- Micro and Macroeconomic dynamics
- Numerical methods for economic dynamic

Session
Nonlinear Dynamics for Economics, Finance and Social Sciences

On the Statistical Significance of Quantile Connectedness Indexes

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We propose a procedure for the evaluation of the statistical significance of the quantile connectedness index developed by [1]. Our approach builds on a simulation-based procedure that allows detecting if the connectedness index built with median quantile regression differs from the index recovered in the tails. In addition, we verify by means of a Monte Carlo experiment the behaviour characterizing the quantile connectedness indexes varying the spillover contribution due to the presence of unconditional correlation and that associated with dynamic interdependence. An empirical example completes our analyses and demonstrates the advantages of the proposed approach.

References

[1] T. Ando, M .Greenwood-Nimmo, and Y. Shin, Quantile Connectedness: Modeling Tail Behavior in the Topology of Financial Networks *Management Science*, 2022.

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Session
Nonlinear Dynamics for Economics, Finance and Social Science

A Discontinuous Model of Exchange Rate Dynamics with Sentiment Traders

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In the present paper, we investigate the complex dynamics arising from a behavioral exchange rate discontinuous model with heterogeneous agents. Unlike previous works explaining the emergence of chaos in the exchange rate models as the resulting of nonlinearity, our model is able to produce endogenous exchange rate dynamics due to the presence of discontinuity induced by a sentiment index relying on [1]. The sentiment index affects the way investors take their trading decisions. In particular, it affects the level of optimism/pessimism of fundamentalists regarding their perception on the value of fundamental. Moreover, it also affects the strength to which one kind of chartists places her buying/sellingcorders. We show that our model, represented by a two-dimensional discontinuous map, has the ability to produce interesting endogenous exchange rate dynamics. In addition, when each component of the map is buffeted by a stochastic component, the model closely replicates the stylized facts of the EUR/USD and EUR/JPY exchange rate markets.

References

[1] S. Manzan and F. Westerhoff. Heterogeneous expectations, exchange rate dynamics and predictability, *Journal of Economic Behavior & Organization*, 64(1):111-128, 2007.

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Session
Nonlinear Dynamics for Economics, Finance and Social Sciences

Border Collision Bifurcations in a Piecewise Linear Duopoly Model

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We consider a duopoly model characterized by a two-dimensional noninvertible continuous map T given by piecewise linear functions, with several partitions, defining a duopoly game. The structure of the game is such that it has separate second iterate so that its dynamics can be studied via a one-dimensional composite function, that is piecewise linear with multiple partitions in which the definition of the map changes. The number of partitions may change from 2 to 5, depending on the parameters. The dynamics are characterized by degenerate bifurcations and border collision bifurcations, which are typical in maps having kink points. Here the peculiarity is the multiplicity of the partitions, which leads to bifurcations different from those occurring in maps with only one kink point. We show several bifurcations, coexistence of cycles, attracting and superstable, as well chaotic attractors and chaotic repellors, related to the outcome of particular border collision bifurcations.

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Session
Nonlinear Dynamics for Economics, Finance and Social Sciences

Dynamics of a Two-class Growth Model with Optimal Saving and Switch in Behavior

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We consider a two-class growth model with optimal saving and switch in behavior [1]. The dynamics of this model is described by a two-dimensional (2D) discontinuous map. We obtain stability conditions of the border and interior fixed points (known as Solow and Pasinetti equilibria, respectively) and investigate bifurcation structures observed in the parameter space of this map, associated with its attracting cycles and chaotic attractors. In particular, we show that on the x-axis, which is invariant, the map is reduced to a 1D piecewise increasing discontinuous map, and prove the existence of a corresponding period adding bifurcation structure issuing from a codimension-two border collision bifurcation point. Then, we describe how this structure evolves when the related attracting cycles on the x-axis lose their transverse stability via a transcritical bifurcation and the corresponding interior cycles appear. In particular, we show that the observed bifurcation structure, being associated with the 2D discontinuous map, is characterized by multistability, that is impossible in the case of a standard period adding bifurcation structure.

References

[1] I. Sushko, P. Commendatore, I. Kubin, *Codimension-two border collision bifurcation in a two-class growth model with optimal saving and switch in behavior*, Nonlinear Dynamics 102, 1071–1095, 2020.

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Session
Nonlinear Dynamics for Economics, Finance and Social Sciences

Waveform Dictionaries and Gabor/wavelet Expansions in Finance

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In economics, important patterns in a process of interest are obscured by noise, for example, liquidity trades, agent errors, unobserved heterogeneity, etc. Managing noise leads to interesting mathematical problems. An example is *denoising* a signal that is a step function (piece-wise constant) with many jumps or discontinuities (also known as breaks and singularities) and contaminated by a noisy process. In this context, the commonly held assumption of stationarity is violated, which leads to the unraveling of theoretical guarantees based on this assumption. One consequence is noisy points being falsely characterized as a discontinuity of the signal. The effects of falsely attributing discontinuities in asset returns could mislead forecasting and statistical inference on the jump points.

Our approach is through assuming the signal we are interested in is a step function and forms another step function based on a sample generated by this signal. Then we remove noise from the data-derived step function through a sub-class of greedy algorithms known as the Weak-Orthogonal Greedy Algorithm (WOGA) or matching pursuit (MP). The algorithm does this by selecting an elementary function from a highly redundant set that is most collinear to the current iterations step function, producing a residual that is carried over to the next step to apply the optimization once again. Execution of the matching pursuit will then produce an approximate orthogonal basis expansion of the signal of interest after a desired number of iterations with these selected elementary functions. The highly redundant set that is used in the MP is referred to as a dictionary and the choice of one is guided by the sought-after properties of the signal. We select the waveform dictionary of a rectangular window function to capture discontinuities, which contains all the translations, scaling, and modulations of the window function. We proved that with the smaller wavelet dictionary, a set of coefficients that produce an approximate orthogonal expansion with dictionary elements can be iteratively constructed in polynomial time. In addition, the expansion is simple to interpret as it is a step function with the average of terms in the sample over the support of the different steps.

SS10 - NONLINEAR WAVES

Special Session

Organizer: Thiab Taha

This session will focus on computational and theoretical aspects of nonlinear wave phenomena. Interdisciplinary aspects of the subject will be emphasized, as well as the interaction between computation, theory and applications.

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Session
Nonlinear Waves

A Global Characterization of Steady Periodic Waves over a Flat Seabed

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Basing on the integral equation of Byatt-Smith [1], a semi-analytical iterative scheme is proposed to describe steady periodic waves propagating over a flat seabed in all the regimes of motions (namely, in deep, intermediate and shallow water conditions). The definition of the iterative scheme is achieved along with a detailed study of the geometrical wave parameters. This part is aimed at the derivation of a global scaling allowing for a consistent representation of the wave dynamics in all the regimes of motion. Comparisons with the existing fifth-order theories for wave propagation show that the proposed model is accurate in all the regimes of motion and that it does not present any of the limitations affecting the Stokes and cnoidal wave solutions in shallow- and deep-water conditions respectively. Further, the proposed scheme also provides a reliable approximation of the dynamics of maximum amplitude waves.

Finally, some possible applications of the proposed scheme are shown. In particular, the iterative scheme is used for the validation of numerical models for wave propagation and for the implementation of periodic inflow signals.

References

[1] G.B. Byatt-Smith. *An exact integral equation for steady surface waves.* Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences, 315(1522):405-418, 1970. ISSN 0080-4630.

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Session
Nonlinear Waves

Stability of Fronts in the Diffusive Rosenzweig-MacArthur Model

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We consider a diffusive Rosenzweig-MacArthur predator-prey model in the situation when the prey diffuses at the rate much smaller than that of the predator. The existence of fronts in the system was proved in [1] using Geometric Singular Perturbation Theory. The underlying dynamical system in a singular limit is reduced to a scalar Fisher-KPP equation and the fronts supported by the full system are small perturbations of the Fisher-KPP fronts. The current project is focused on the stability of the fronts. In particular, it is of interest whether the stability of the fronts is also governed by the scalar Fisher-KPP equation. The techniques of the analysis include a construction of unstable augmented bundles and their treatment as multiscale topological structures.

References

[1] H. Cai, A. Ghazaryan, and V. Manukian. *Fisher-KPP dynamics in diffusive Rosenzweig-MacArthur and Holling-Tanner models.* Math. Model. Nat. Phenom. **14** (2019), no. 4, Paper no. 404, 21 pp.

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Session
Nonlinear Waves

Stripe Pattern Formation in PNP Steric Model

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Poisson-Nernst-Planck (PNP) equations have been frequently used to describe the distributions of electric potential, ion concentrations in ionic solutions. However, classic PNP equations treat ion as a point without volume, which can be inadequate for highly concentrate ionic solutions like ionic liquids. Several modifications on adding finite-size effect into PNP equations have been proposed in literatures. We have developed our own version of that called PNP steric model [1] by adding chemotaxis-like nonlinear intra- and inter-diffusion terms into Nernst-Planck equations with an additional bi-Laplacian diffusion term to suppress high-mode instability. By fixing inter-diffusion coefficient and varying intra-diffusion coefficient, we found the formation of steady-state stripe pattern in cation and anion concentration distributions, which represents a trough-and-peak concentration distribution caused by inter-diffusion repulsion and electrostatic attraction. With further decreasing of intra-diffusion coefficient, the steady-state stripe pattern becomes unstable and evolves to curve stripes even to a complicated dynamic stripe pattern with dislocations happening during evolution.

References

[1] T.L. Horng, T.C. Lin, C. Liu, and B. Eisenberg, PNP equations with steric effects: A model of ion flow through channels, J. Phys. Chem. B, 116(37), 11422–11441, 2012.

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Session
Nonlinear Waves

Lagrangian Dynamics of Nonlinear Waves in Shallow-water Systems, Including Rotation, Baroclinicity, and Mean Flows

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We rewrite both hydrostatic and non-hydrostatic equations of barotropic (one-layer) and baroclinic (two-layer) rotating shallow water systems in Lagrangian form using as dynamical variables the fluid columns displacements in one layer configuration, and these displacements in the lower layer in two-layer configuration. We look for solutions in form of weakly nonlinear plane-parallel, respectively surface and internal, inertia-gravity waves assuming that rotation is weak. Rotation necessitates introduction of the transverse to the direction of the wave propagation velocity. As usual, homogeneous linear wave equations arise in the lowest order, and removal of secular terms in the next order leads to modulation equations. We show that Lagrangian variables allow for a straightforward introduction of means, in addition to oscillating wave variables. We also admit a nonzero time-dependent overall mass flux in the two-layer system, which is traditionally set to zero in the literature.

In both one- and two- layer systems in *hydrostatic configuration without rotation* we get simple-wave equations exhibiting wave-breaking in finite time. In *non-hydrostatic configuration without rotation* we get KdV equation with celebrated soliton solutions. If a slow overall mass flux (a "tide") through the system is present, it gives a time dependent source producing modulations in the soliton propagation. In *hydrostatic configuration with rotation* we get fully integrable, yet producing wave-breaking for some initial conditions, Ostrovsky-Hunter equation. In *non-hydrostatic configuration with rotation* we get in both systems the Ostrovsky equation. If the mean Lagrangian displacement is present, it is subject to *inertial oscillations* superimposed onto nonlinear waves. Unlike the non-rotating case, an overall mass flux with nonzero fast-time average in the two-layer system turns to be incompatible with the setup, as it leads to a secular growth of the transverse velocity due to the Coriolis force.

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Session
Nonlinear Wave

Integrable Nonlinear Wave Equations and Painlevé Hierarchies

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The question of obtaining analogues of the Painlevé equations, having properties that mirror those of the Painlevé equations themselves, is a topic that has been of interest for some considerable time now. In particular, the derivation of sequences of such ordinary differential equations, of increasing order, that is, of so-called Painlevé hierarchies, is a subject that has attracted significant attention. In this regard, use is made of the well-known connection with completely integrable systems. However, the underlying structures of integrable systems have also been shown to play a crucialrole in extracting information about the properties of the Painlevé hierarchies thus obtained. Important properties include auto-Bäclund transformations and special integrals, as these provide a means of constructing sequences of solutions.

Here we consider examples of the construction of Painlevé hierarchies, and of thederivation of auto-Bäcklund transformations and special integrals. As indicated above, of fundamental importance in obtaining these results are the properties ofrelated hierarchies of completely integrable equations. Further related equations and other properties are also discussed.

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Session
Nonnlinear Wave

Numerical Methods for Solving Nonlinear Evolution Equations

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In this talk a survey and a method of derivation of certain class of numerical schemes and an implementation of these schemes will be presented. These schemes are constructed by methods related to the Inverse Scattering Transform (IST) and can be used as numerical schemes for their associated nonlinear evolution equations. They maintain many of the important properties of their original partial differential equations such as infinite numbers of conservation laws and solvability by IST. Numerical experiments have shown that these schemes compare very favorably with other known numerical methods.

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Session
Nonlinear Waves

Construction of Solitary Wave for Fractional KdV Equation with Inhomogeneous Symbol

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In this work, we consider fractional Korteweg-De Vries equation with an inhomogeneous symbol

$$u_t + (\Lambda^{-s}u + u^2)_x = 0, \quad s \in (0,1)$$

where $\Lambda^{-s}u = \mathcal{F}^{-1}\big[(1+|\xi|^2)^{-\frac{s}{2}}\hat{u}(\xi)\big]$. The construction of solitary waves for corresponding equation is based on parameterising the solution curves through relative wave height and applying a limiting argument. The obtained branch evolves from zero solution, traverses unique points in the wave speed-wave height space, and reaches a singular highest wave at $\varphi(0) = \dfrac{\mu}{2}$. A uniform estimate is employed with the limiting arguments, and the Galilean transform is showed to exclude vanishing waves and waves at negative surface depth. The periodic waves converge locally uniformly to a wave with negative tails, and this is transformed to the desired branch of solutions.

SS11- RECENT ADVANCES IN DATA SCIENCE. COMPUTATIONAL ASPECTS AND APPLICATIONS

Special Session

Organizer: Christian Acal

Developing models that will be used to address problems of great social impact based on the analysis and decision making (data-driven) is one of the main challenges facing the statistical scientific community at present. This fact together with the advances in computer technology and statistical software have caused that data science is changing rapidly in the last decades. This session aims to gather researchers to present advances in the relevant fields of statistics in order to foster a favourable environment to exchange information and open new collaboration lines.

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Session
Recent Advances in Data Science. Computational Aspects and Applications

Function-on-function PLS Regression: a Penalized Approach

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Functional data analysis is a growing field of research dealing with data observed on a continuum. Specifically, we are interested on the function-on-function linear regression model, where both the response and the predictor are functions. Most contributions to this topic are focused mainly on improving the prediction accuracy of the fitted model. In that sense, our contribution aims to improve, at the same time, both the prediction ability and the interpretability of the estimated parameter function. To this end, a penalized version of the partial least squares regression has been developed to the function-on-function linear regression model, which imposes smoothness on the PLS weights, affecting the smoothness of the resulting parameter function. The good performance of the penalized function-on-function PLS regression is proved in a simulation study, where the results are compared to the non-penalized approach proposed in [1]. The results show a higher accuracy of pFFPLS in predicting the response and in estimating the true coefficient function from which the data were generated.

References

[1] Preda, C. and Schiltz, J. *Functional PLS regression with functional response: the basis expansion approach*, In Fagerberg, J., Mowery, D. C., and Nelson, R. R., editors, Proceedings ASMDA 2011: 14th Applied Stochastic Models and Data Analysis Conference, June 2011, pages 1126-1133. Università di Roma La Spienza, Roma, 2011.

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Session
Recent Advances in Data Science. Computational Aspects and Applications

Robust Estimation and Testing for Step-stress Experiments under Interval Censoring

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Censoring frequently occurs in reliability and survival experiments. Interval censored data occurs in reliability tests when failure times are only known to lie within an interval, but the exact time of failure cannot be directly observed. The censoring problem is particularly relevant for devices that are highly reliable with long lifetimes, requiring extensive experimentation time to make accurate inference under normal operating conditions. An alternative approach is to conduct accelerated life tests (ALTs) by subjecting devices to increased stress factors, causing failure and shortening their lifetimes. The, after suitable inference, the results can be extrapolated to normal conditions. Step-stress ALT designs gradually increase the stress levels at which devices are tested at fixed intervals throughout the experiment. Classical estimation methods using the likelihood function of the lifetime distribution can be highly influenced by data contamination, and consequently any test static based on the maximum likelihood estimator. In this work, we propose a family of robust estimators based on the density power divergence that can handle interval censored data in step-stress experiments. Furthermore, a generalization of the widely used Wald-type test statistic for testing composite null hypothesis is defined from these robust estimators. Finally, a simulation study empirically illustrates the claimed robustness of the estimators and test statistics.

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Session
Recent Advances in Data Science. Computational Aspects and Applications

A Spatial Functional Regression Approach from Correlated Curves in Space

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This paper deals with spatial functional multiple regression in Hilbert spaces, in the case where the response, and the error term are spatial Gaussian stochastic processes with values in a separable Hilbert space. The kernel regressors take their values in the space of Hilbert-Schmidt operators. We restrict our attention to the case where the error term is a SARH(1) process (Spatial Autoregressive Hilbertian process of order one). The proposed approach is applied to the statistical analysis of COVID-19 pandemic data.

Keywords: Functional regression, SARH(1) process, spatial functional analysis of COVID-19 pandemic data.

References

[1] Bosq D. *Linear Processes in Function Spaces.* Springer-Verlag, New York (2000).

[2] Ruiz-Medina, M. D., Miranda, D., and Espejo, R. M. *Dynamical multiple regression in function spaces, under kernel regressors, with ARH (1) errors.* Test, 28 (2019): 943-968.

[3] Ruiz–Medina, M. D., and Miranda, D. *Bayesian surface regression versus spatial spectral nonparametric curve regression.* Spatial Statistics, 50 (2022): 100604.

[4] Ruiz-Medina M.D. *Spatial functional prediction from spatial autoregressive Hilbertian processes.* Environmetrics 23, (2012b):119–128

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Session
Recent Advances in Data Science. Computational Aspects and Applications

How to Model a Complex System Subject to Multiple Events and a Vacation Policy in a Matrix-computational Form. MMAPs

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One of the main problems when modeling a complex system in reliability is to develop the methodology in an algorithmic and computational way that eases the computational implementation and the interpretation of the results. This problem is solved when MMAPs are considered. This work analyses a complex multi-state cold standby system subject to multiple events and a a vacation policy. Preventive maintenance and loss of units are considered. The online unit may undergo internal and external failure and multiple levels of degradation are considered. The levels of degradation are observed through random inspections and, in case of major damage, the unit is taken to the repair facility where a preventive maintenance process is carried out. Therefore two types of tasks are performed by the repairperson, corrective repair and preventive maintenance. Several performance measures are built, through analytical-matrix methods, for transient and stationary regime. Rewards are included and an analysis performace-cost is carried out.

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References

[1] M.F. Neuts, A versatile Markovian point process. *Journal of Applied Probability*, 16, 4, 764-779, 1979.

[2] J.E. Ruiz-Castro, Optimizing a multi-state cold-standby system with multiple vacations in the repair and loss of units. *Mathematics*, 9, 8, 913, 2021.

[3] J.E.. Ruiz-Castro and Ch. Acal, MMAPs to model complex multi-state systems with vacation policies in the repair facility. *Journal of Reliability and Statistical Studies*, 15, 2, 47-504, 2022.

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Session
Recent Advances in Data Science. Computational Aspects and Applications

Wavelet-based Sparse Optimization via Fixed-point Iteration Scheme in High-dimensional Data Analysis

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It has been argued that in the small n large p setting, often called 'wide' data, sparsity is meant to be reinforced to detect interpretable low-dimensional structures with statistical significance [1]. Therefore, finding a balance between sparsity and other statistical properties (e.g. independence) is of particular interest to address the dimensionality reduction problem in complex wide data. Here, we combine wavelet analysis techniques to find a suitable sparse subspace representation in the sense of the temporal structure of the data along with a posterior optimization via fixed-point iteration schemas performed on isotropic data derived from the inter-subject (or spatial) structure of these wavelet expansions. This last procedure is conducted across multiple levels of smoothing generated in the wavelet transform via factorization of the original space into a sequence of non-linear subspaces that are maximally sparse and statistically independent. Using multiresolution analysis, estimators can be computed extremely fast because the inverse of the dyadic wavelet transform is computed in $\mathcal{O}(2^J)$ operations, and the subsequent optimization with fixed-point iteration requires reasonably low-computational complexity. We show the properties of our method through different whitening and wavelet estimators, and apply our method to EEG data for artifact detection and source localization.

References

[1] Bickel, P.J., Kur, G., & Nadler, B. *Projection pursuit in high dimensions.* Proceedings of the National Academy of Sciences, 115, 9151-9156, 2018.

[2] Vidal, M., & Aguilera, A. M. *Novel whitening approaches in functional settings.* Stat, 12(1), e516, 2023.

[2]The authors acknowledge the financial support from the project PID2020-113961GB-I00.

SS12 - RECENT ADVANCES IN LATTICE BOLTZMANN METHODS

Special Session

Organizer: Ralf Deiterding

The lattice Boltzmann method (LBM) has become a powerful tool in computational fluid dynamics. A straightforward explicit stream and collide algorithm, ease of parallelization and natural handling of complex geometries have led to the development of a large number of mathematical models within the LBM framework. On the other hand, heterogenous resolution requirements, complex equations of state or subscale models, e.g., for turbulence, are usually more difficult to combine with the mesoscopic LBM than with traditional Navier-Stokes-based fluid solvers. This mini-symposium will bring together researchers working on and with the LBM in the widest sense and include contributions in the development of new lattice Boltzmann type schemes and models as well as advanced engineering applications.

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Session
Recent Advances in Lattice Boltzmann Methods

Non-Cartesian Lattice Boltzmann Methods with Structured Adaptive Mesh Refinement

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The standard lattice Boltzmann method is formulated for equally spaced Cartesian grids, which makes it computationally expensive in practical aerodynamics. Here, we discuss an alternative approach solving the two-dimensional discrete-velocity Boltzmann equation in generalised curvilinear coordinates with an effective dissipation-stabilized central finite difference scheme. The generalised LBM resolves large gradients in the wall vicinity with considerable fewer mesh points, as will be demonstrated by aerodynamical benchmarks of laminar flow around cylinders and aerofoils [1]. Incorporated into our fully parallelised finite-volume framework AMROC, that uses a block-structured adaptive mesh refinement in addition, the proposed methodoloy is highly efficient. Various test cases, including convective heat transfer flows, will be used to demonstrate its performance and accuracy [2].

References

[1] J. A. Reyes Barraza, R. Deiterding. Towards a generalised lattice Boltzmann method for aerodynamic simulations, *J. Computational Science* 45: 101182, 2020.

[2] J. A. Reyes Barraza, R. Deiterding. A curvilinear lattice Boltzmann scheme for thermal flows. *Mathematics and Computers in Simulation* 202: 405-420, 2022.

Session
Recent Advances in Lattice Boltzmann Methods

Lightweight Lattice Boltzmann

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An enhanced variant of the lattice Boltzmann method is presented to efficiently simulate bi-component systems. Unlike traditional methods, this approach reconstructs the distribution functions using hydrodynamic variables (density, momentum, and pressure tensor) without the need to store the complete set of discrete populations. As a result, this technique exhibits reduced memory usage and data access overheads. Various benchmark tests relevant to soft matter, such as fluid droplet collisions, are conducted to validate the effectiveness of the method. These findings hold promise for the high-performance simulation of soft matter systems on forthcoming exascale computers [1].

References

[1] A. Tiribocchi, A. Montessori, G. Amati, M. Bernaschi, F. Bonaccorso, S. Orlandini, S. Succi, M. Lauricella, *Lightweight Lattice Boltzmann*, J. Chem. Phys. 158, 104101 (2023).

SS13 – TRIANGULATIONS, MESHING AND APPLICATION

Special Session

Organizers: Miguel Padron, Jose Pablo Suarez Rivero

Meshing and Triangulation are used today in many area as Graphics, Engineering simulations, and Modelling. Nowadays discrete geometry of meshes and triangulation is the key to understand huge advances in fields as physics, mathematics and engineering.

In science and engineering applications, triangular, quadrilateral and polyhedral meshes in both 2D and 3D are commonly used for Finite Element and Volume Analysis, Computational Geometry, CAD, Surface and Solid Modelling, Parametric, Adaptive mesh refinement, Constraint-based and Feature Modelling, discretization and Engineering Simulations, Meshing for High-Performance and Distributed Computing, Algorithms and neural networks methods in discretizations. Contributions may also cover theoretical aspects of Meshing and Triangulation.

Although main topics could cover construction of quality triangulations of simplices in n dimensions authors are invited to send contributions with focus in the research and development of Delaunay and optimal methods, Mesh Generation and post-processing, n-dimensional subdivision methods, smoothing and optimization among others.

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Session
Triangulations, Meshing and Applications

Near Equilateral Tetrahedra and the Convergence into Less Than 37 Similarity Classes

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In 1983, Adler [1] mentioned that if a tetrahedron is nearly equilateral (edge lengths are within 5% of each other) and the second longest edge is opposite to the longest one, then the new subtetrahedra generated by the iterative longest edge bisection (LEB) falls into less than or equal to 37 similarity classes. This has been over more than 30 year the Adler's conjecture.

In this work, we focus on different scenarios where the LEB of nearly equilateral tetrahedron falls into less than 37 classes. We study the different forms of convergence, showing that not all numbers between 1 to 36 can be achieved but 8, 9, 13, and 21 are possible. This improves the Adler [1] work by giving more details of the similarity classes generated in the LEB of near equilateral tetrahedra. For this purpose, an edge-based representation of tetrahedra is given for checking the new similarity classes generated by the LEB [2].

References

[1] A. Adler. On the bisection method for triangles. *Math. Comp.* **40** (1983), 571–574.

[2] J. P. Suárez, A. Trujillo, T. Moreno. Computing the exact number of similarity classes in the longest edge bisection of tetrahedra *Mathematics* **9**(12) (2021), 1447.

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Session
Triangulations, Meshing and Applications

Compact and Efficient Data Structure for the Study of LEB of Tetrahedra

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In the end of the eighties emerged the algorithms and data structures for mesh generation and Finite Element method, [1]. And still today it seems a great advance to improve the computations aspects to attack the increasing complexity such as mesh dimensions or number of elements.

We introduce an edge-based representation of tetrahedra in the form of a sextuple of real values that is quite efficient for computing the similarity classes generated by the LEB (Longest Edge Bisection). Although edge-based data structure are not new in the context of mesh generation, less attention have been given to the application of similarity classes computations.

We use the edge-based representation to study a problem that still remains open in the LEB: whether the iterative LEB of tetrahedra produces a finite number of new shape classes or not.

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References

[1] A. Adler. On the bisection method for triangles. *Math. Comp.* **40** (1983), 571–574.

SS14 - USING BLOCK METHODS FOR SOLVING DIFFERENTIAL PROBLEMS

Special Session

Organizer: Higinio Ramos

In everyday life, Machine Vision has made significant progress toward becoming more pervasive due to recent developments in artificial intelligence and computing capabilities. Despite the tangible and excellent results, the current Machine Vision techniques fall short of our expectations compared to the ease with which the Human Visual System (HVS) deals with complex scene analysis and abstraction. Thus, we are witnessing a growing interest in HVS-inspired approaches for developing more thoughtful and efficient visual information modeling and processing methods. The Mini-Symposium aims to bring together leading scientists to present their latest HVS-inspired practices and to establish new directions for future investigations and cooperation. We welcome contributions using tools including (but not restricted to): Applied Harmonic Analysis, Compression Methods, Geometric and Topological Techniques, Mathematical Morphology, Partial Differential Equations, Probabilistic and Statistical Methodologies, Interpolation Methods, Multiresolution Analysis, and Variational Methods for applications related to Signal and Image Processing, Pattern Recognition, and Visual Machine Learning

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Session
Using Block Methods for Solving Differential Problems

Adaptive Stepsize Optimized Three-step Hybrid Block Method for First-order Initial Value Problems

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In this work, an efficient numerical solver based on the hybrid optimized block method is designed and analyzed for the approximation of solutions of first-order initial value problems. The scheme is designed in such a way that each block contains three steps with three offset points. In order to further improve the approximations, a simpler formulation of the formulas that constitute the method were also introduced and the step sizes were made variable by adapting them based on a local error estimate. The region of stability and the order of accuracy of the formulas in the method were shown, as well as the convergence of the method. The efficiency of the proposed strategy was demonstrated by employing it to solve some selected problems.

References

[1] W.E. Milne, *Numerical solution of differential equations*, New York: Dover, 1970.

[2] M.O. Ogunniran, Y. Haruna, R.B. Adeniyi, M.O. Olayiwola, *Optimized Three-step Hybrid Block Method for Stiff Problems in Ordinary Differential Equations*, Çankaya University Journal of Science and Engineering 17(2) 80-95, 2020.

[3] H. Ramos, Z. Kalogiratou, Th. Monovasilis, and T.E. Simos. *An optimized two-step hybrid block method for solving general second order initial-value problems*, Numerical Algorithms 4(72) 1089–1102, 2016.

[4] L. Brugnano and D. Trigiante, *Solving differential equations by multistep initial and boundary value methods*, CRC Press, 1998.

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Session
Using Block Methods for Solving Differential Problems

An Optimized Algorithm for Numerical Solution of Coupled Burgers Equations

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Investigation of the solutions of the coupled viscous Burgers system is crucial for realizing and understanding some physical phenomena in applied sciences. Particularly, Burgers equations are used in the modeling of fluid mechanics and nonlinear acoustics. In the present study, a modified meshless quadrature method based on radial basis functions is used to discretize the partial derivatives in the spatial variable. A high resolution optimized hybrid block method is then used to solve the problem in the temporal variable. To validate the proposed method, several test problems are considered and the simulated results are compared with exact solutions and previous works. The unconditional stability of the proposed algorithm is verified.

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Session
Using Block Methods for Solving Differential Problems

The Semi-implicit EM Method for Nonlinear Non-autonomous SDEs Driven by a Class of Lévy Processes

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In this talk, we investigate the strong convergence of the semi-implicit Euler-Maruyama (EM) method for stochastic differential equations with non-linear coefficients driven by a class of Lévy processes. The dependence of the convergence order of the numerical scheme on the parameters of the Lévy processes is discovered, which is different from existing results. In addition, the existence and uniqueness of numerical invariant measure of the semi-implicit EM method is studied and its convergence to the underlying invariant measure is also proved. Numerical examples are provided to confirm our theoretical results.

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Session
Using Block Methods for Solving Differential Problems

Block θ-methods for DAEs and DDAEs

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In this talk, a class of block θ-methods is proposed for solving differential-algebraic equations and delay differential-algebraic equations. We first establish convergence and asymptotic stability of the block θ-methods applied to index 1 and 2 differential-algebraic equations. For delay differential-algebraic equations, to preserve the one-step nature and avoid extra evaluations of the right-hand side function, we use the continuous extension of the discrete solution to provide an approximation of the delayed term. It is shown that the block θ-methods for delay differential-algebraic equations retain the same convergence order as for delay-free problems. We fortunately prove that the coefficient matrices of the block θ-method and its continuous extension can be upper triangulated simultaneously, which plays a crucial role in the asymptotic stability analysis of the block θ-methods. A sufficient and necessary condition for asymptotic stability of the block θ-method applied to linear delay differential-algebraic equations is achieved. Finally, some numerical experiments are performed to confirm the convergence and stability results of the proposed block θ-methods.

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Session
Using Block Methods for Solving Differential Problems

A New Block Method for Direct Integration of Third-order BVPs

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This proposed talk will introduce an efficient hybrid block method for directly solving third-order boundary value problems (BVPs). The proposed method will be developed by considering three intermediate points, and a suitable polynomial will be used to approximate the theoretical solution of the BVPs under consideration. The fundamental properties of the proposed method, including convergence order and stability, will be theoretically analyzed. Some test problems, including boundary layer problems and other physical model problems, will be numerically solved to determine the efficiency and utility of the proposed method in applied sciences and engineering.

POSTERS

Randomized GSVD Based Regularization for the Inverse Problem of Ultrasound Tomography

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Ill posed inverse problems $\mathbf{Xy} = \mathbf{b}$ arise in various fields of science and technology. We are particularly interested in the inverse problem of ultrasound tomography (UT), since it is a noninvasive medical imaging modality which can be used for breast cancer detection. To solve the aforementioned problem, the Tikhonov regularization method in general form combined with algorithm for parameter selection is poposed in [1]. While this method is more effective for UT than comparable iterative regularization method, there is still a question of time efficiency. The part of the method responsible for its slower execution is the calculation of generalized singular value decomposition (GSVD) of matrix pair $(\mathbf{X}, \mathbf{L})$, where $\mathbf{L}$ is the regularization matrix. One idea to speed up the process is to use randomized algorithms for approximation of GSVD instead of calculating full GSVD [2]. In this talk we present new randomized GSVD version of the regularization algorithm for the inverse problem of UT. It is because of randomized algorithms, while its efficiency in regularization is comparable to the method from [1]. Aforementioned methods are tested using numerical simulation of UT.

References

[1] A. Carević, I. Slapničar and M. Almekkawy, *Solving UT's Inverse Problem: Automating Regularization Parameter Selection*, IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control, 69.8 (2022): 2447-2461

[2] Y. Wei, P. Xie and L. Zhang, *Tikhonov regularization and randomized GSVD*, SIAM Journal on Matrix Analysis and Applications, 37.2 (2016)

Approximating Inter-arrival Distribution by Phase Type Distribution: Asymmetric Kernel Method

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In our work, we are interested in the approximation of a class of queueing systems through the replacement of their inter-arrival distributions by phase type distributions. We consider the approximation of GI/M/1 queueing system by a PH/M/1 system. We propose the nonparametric asymmetric kernel method in the study of strong stability of the PH/M/1 queuing system.

References

[1] S. Asmussen, Applied probability and queues. 2nd edn. Springer, New York, 2003.

[2] Y. Djabali, Stablité Forte dans les systèmes d'Attente de type Phase: Cas des Systèmes PH/M/1 et M/PH/1. Thèse de Doctorat, Université de Bejaia, Algérie, 2017.

[3] M. Hirukawa, M. Sakudo, Family of the generalised gamma kernels: a generator of asymmetric kernels for nonnegative data. Journal of Nonparametric Statistics 27, 41- 63, 2015.

Observer-based Dissipativity of Parabolic Systems with Multiple Actuators and Time Delays[3]

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This research paper investigates the observer-based dissipativity analysis of partial differential equations (PDEs) of parabolic type with time-varying delays. Specifically, the study focuses on second-order PDEs with external disturbances. The goal is to establish sufficient conditions that ensure the asymptotic stability and strict dissipativity of the considered system. To enhance the system's reliability and performance, the output is measured at multiple points in this study. By dividing the spatial domain into smaller sub-domains, the system employs multiple actuators and controllers that target specific components. This approach provides locally averaged measurements within each sub-interval, resulting in a more efficient and reliable system. The effectiveness of the developed approach is verified through numerical examples, demonstrating its potential for practical applications.

References

[1] E. Fridman and Y. Orlov, An LMI approach to H_∞ boundary control of semi linear parabolic and hyperbolic systems, *Automatica* 45(9) (2009) 2060-2066.

[2] R. Lozano, *et al*., *Dissipative systems analysis and control: theory and applications communications and control engineering*, Springer, (2000).

[3] Z.P. Wang, H.N. Wu and H. X. Li, Fuzzy Control Under Spatially Local Averaged Measurements for Nonlinear Distributed Parameter Systems With Time-Varying Delay, *IEEE Tr. Cybern.* 99 (2019) 1-11.

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